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Mechanical Bonds and Topological Effects in Radical Dimer Stabilization

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SUPPORTING INFORMATION

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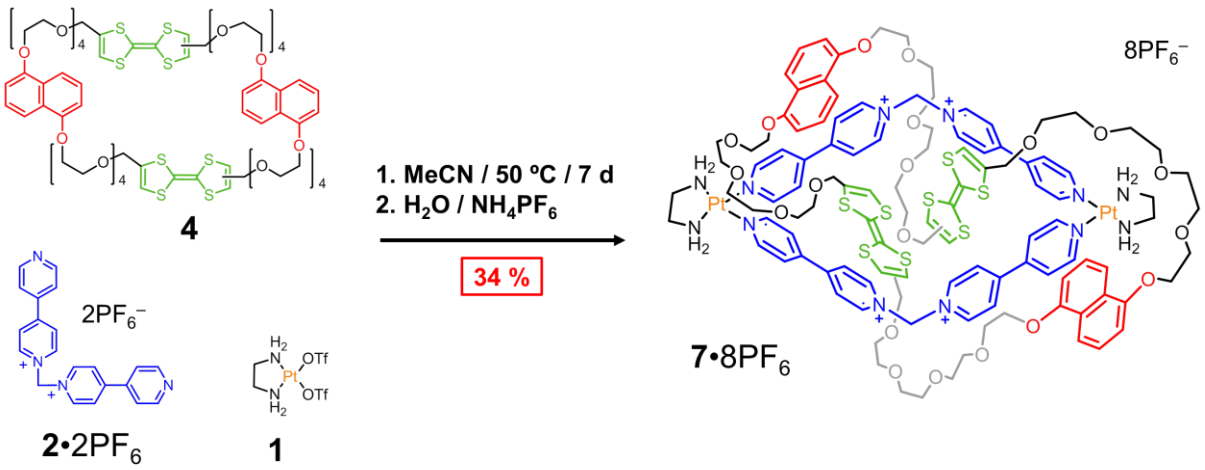
Section A. Materials / General Methods / Instrumentation

All reagents were purchased from commercial suppliers (Aldrich or VWR) and used without further purification. Crown ether [S1] **4** contains four alternating π-electron rich TTF and DNP units, the TTF and DNP macrocycle[S2] **3** and the ligand[S3] **2**·2PF_6 were prepared according to literature procedures. Thin layer chromatography (TLC) was performed on silica gel 60 F254 (E. Merck). UV–Vis–NIR Absorbance spectra were recorded using a Varian 100-Bio UV/Vis spectrophotometer. Nuclear magnetic resonance (NMR) spectra were recorded at 298 K on Bruker Avance 500 and 600 spectrometers, with working frequencies of 500 and 600 MHz for ^{1}H, and 125 and 150 MHz for ^{13}C nuclei, respectively. Chemical shifts are reported in ppm relative to the signals corresponding to the residual non-deuterated solvents.[S4] All ^{13}C spectra were recorded with the simultaneous decoupling of proton nuclei. High-resolution mass spectra were measured on an Agilent 6210 Time of Flight (TOF) LC-MS, using an ESI source, coupled with Agilent 1100 HPLC stack, using direct infusion (0.6 mL min^{-1}). EPR Measurements at X-band (9.5 GHz) were performed with a Bruker Elexsys E580, equipped with a variable Q dielectric resonator (ER-4118X-MD5-W1). All sample preparations were performed in an Argon-filled atmosphere. Samples were loaded into quartz 1.4 mm tubes and sealed with a clear ridged UV doming epoxy (IllumaBond 60-7160RCL) and used immediately after preparation. Steady-state solution CW EPR spectra were collected with a 0.25 G modulation amplitude 2.56 ms time constant, and 10.24 ms conversion time, averaging 100 sweeps 50 G wide, centered around 2465 G. Steady-state solid CW EPR spectra were measured with the same parameters, except for the modulation amplitude, which was 0.05 G. Cyclic voltammetry experiments were performed on a Princeton Applied Research 263 A Multipurpose instrument interfaced to a PC, using a glassy carbon working electrode (0.071 cm^2, Cypress system). The electrode surface was polished routinely with 0.05 μm^2 alumina/water slurry on a felt surface immediately before use. The counter electrode was a Pt coil and the reference electrode was a AgCl coated Ag wire. The concentrations of the samples were 1 mM in 100 mM electrolyte solution ($TBAPF_6$ in MeCN). Spectroelectrochemical (SEC) experiments were carried out using a custom-built optically transparent thin layer electrochemical (OTTLE) cell with an optical path of 2 mm, using a Pt grid as working electrode, a Pt wire as counter electrode and a Ag wire pseudo-reference electrode. Experimental errors: potential values, ±5 mV, absorption maxima, ±1 nm. Single crystal X-ray data were measured on a Bruker Kappa Apex II CCD diffractometer using Cu-Kα radiation. Data collection and structure refinement details can be found in the CIF files. CCDC depositions 952939, 952940, 952941, 965480, 965478, 975035 and 965480 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif

Section B. Synthetic Protocols

1) Molecular Solomon link

1.1) Pt(II) Complex **7**•$8PF_6$

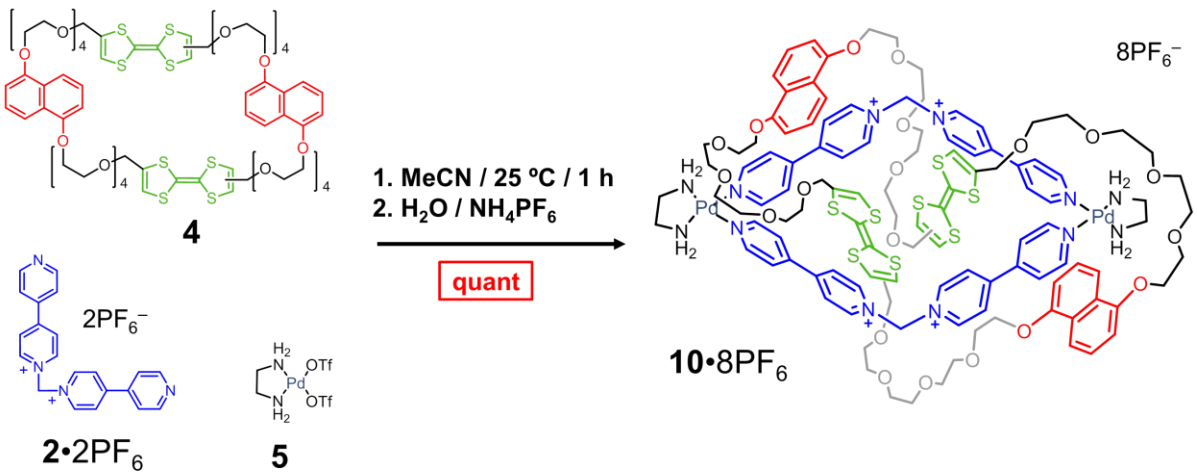


Scheme S1. Synthesis of ***7•8PF$_6$***.

7•8PF$_6$: Ligand **2**·$2PF_6$ (11.0 mg, 7.15 μmol) was added to a solution of the crown ether **4** (10.6 mg, 7.15 μmol) dissolved in MeCN (956 μL), and the mixture was stirred at ambient temperature for 1 h. A 50 mM MeCN solution of ethylenediamineplatinum(II) bis(trifluoromethanesulfonate) **1** (429 μL, 21.5 μmol) was added, and the resulting solution was stirred at 50 °C for 7 days. The crude mixture was purified by preparative TLC (SiO_2, 0.5% NH_4PF_6 in Me_2CO), and dissolved in MeCN. A saturated aqueous solution containing NH_4PF_6 was added and MeCN was removed under reduced pressure. The resultant precipitate was collected by filtration, washed with H_2O, and dried in *vacuo* to give the compound **7**•$8PF_6$ (9.38 mg, 2.47 μmol) as a dark green solid in 34% yield. ^{1}H NMR (500 MHz, CD_3CN, 298 K): δ 9.31 (br, 4H, H_α), 9.13 (d, $^3J_{HH}$ = 6.3 Hz, 8H, H'$_{\alpha+}$ / H'$_\alpha$ (CH_2 / Pt)), 8.54 (d, $^3J_{HH}$ = 6.2 Hz, 4H, $H_{\alpha+}$ (CH_2)), 7.87 (d, $^3J_{HH}$ = 6.8 Hz, 4H, H'$_{\beta+}$ (CH_2)), 7.70 (d, $^3J_{HH}$ = 7.0 Hz, 4H, H_β (Pt)), 7.60 (d, $^3J_{HH}$ = 8.4 Hz, 2H, $H_{4/8}$ (DNP)), 7.54–7.48 (br m, 12H, $H_{\beta+}$ / H'$_{\beta+}$ (CH_2 / Pt), $H_{3/7}$ / H'$_{4/8}$ (DNP)), 7.32 (d, $^2J_{HH}$ = 14.3 Hz, 2H, H_a), 7.28 (t, $^3J_{HH}$ = 8.0 Hz, 2H, H'$_{3/7}$ (DNP)), 7.06 (d, $^3J_{HH}$ = 7.6 Hz, 2H, $H_{2/6}$ (DNP)), 6.76 (d, $^2J_{HH}$ = 14.3 Hz, 2H, H'$_a$),

6.54 (d, $^{3}J_{HH}$ = 7.5 Hz, 2H, H'$_{2/6}$ (DNP)), 5.94 (s, 2H, H_{TTF}), 5.89 (s, 2H, H_{TTF}), 5.80 (br m, 2H, –CH_2NH_2), 5.03–4.74 (m, 10H, –CH_2NH_2 / –OCH_2CH_2–), 4.27–3.37 (m, 56H, –CH_2NH_2 / –OCH_2CH_2–), 2.93–2.72 (m, 12H, –CH_2NH_2 / –OCH_2CH_2–); ^{13}C NMR (125 MHz, CD_3CN, 298 K): δ 155.8 (CH), 155.0 (C), 154.6 (CH), 154.4 (C), 152.2 (C), 150.9 (C), 144.3 (C), 142.6 (C), 140.6 (C), 134.4 (C), 131.7 (C), 127.7 (CH), 127.4 (CH), 126.6 (C), 126.2 (CH), 125.8 (C), 125.6 (CH), 125.3 (CH), 125.0 (CH), 120.0 (CH), 119.1 (CH), 115.3 (CH), 114.2 (CH), 111.1 (C), 108.2 (C), 107.8 (CH), 106.7 (CH), 78.7 (CH_2), 73.5 (CH_2), 72.6 (CH_2), 71.8 (CH_2), 71.5 (CH_2), 71.5 (CH_2), 71.4 (CH_2), 70.8 (CH_2), 70.7 (CH_2), 70.5 (CH_2), 69.9 (CH_2), 69.8 (CH_2), 69.4 (CH_2), 69.1 (CH_2), 68.9 (CH_2), 68.8 (CH_2), 68.5 (CH_2), 48.9 (CH_2), 48.7 (CH_2); HR MS (ESI–TOF) Calcd for $C_{114}H_{140}N_{12}O_{20}Pt_2S_8P_8F_{48}$ (PF_6^- salt): *m*/*z* = 1756.2601 ($[M - 2(PF_6)]^{2+}$), 1122.5185 ($[M - 3(PF_6)]^{3+}$); Found: *m*/*z* = 1756.2610 ($[M - 2(PF_6)]^{2+}$), 1122.5254 ($[M - 3(PF_6)]^{3+}$).

1.2) Pd(II) Complex **10**•8PF_6



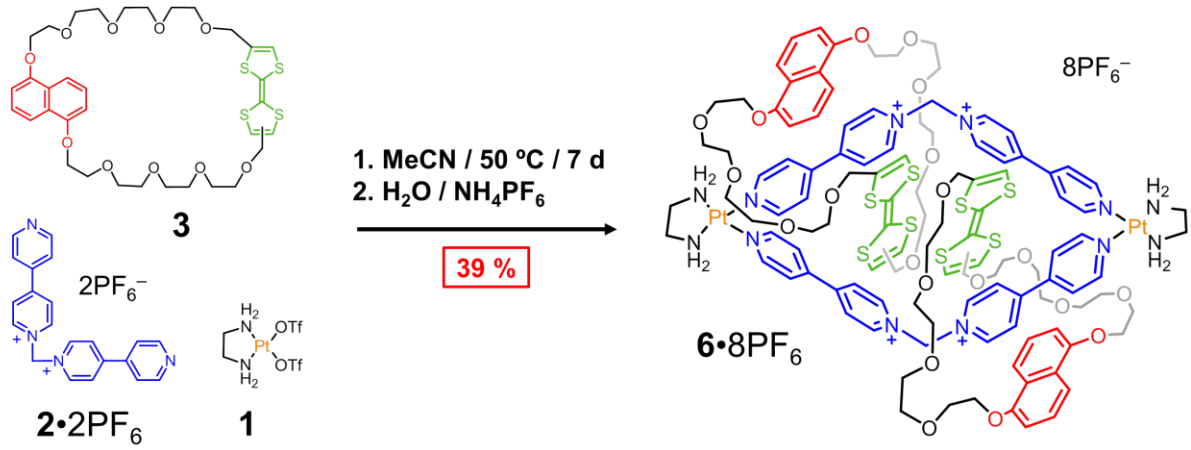
Scheme S2. Synthesis of ***10•8PF$_6$***.

10•8PF$_6$: Ligand **2**·2PF_6 (2.47 mg, 4.00 μmol) was added to a solution of crown ether **4** (2.96 mg, 2.00 μmol) in MeCN (508 μL), and the mixture was stirred at ambient temperature for 1 h. A 50 mM MeCN solution of ethylenediaminepalladium(II) bis (trifluoromethanesulfonate)

5 (92 μL, 4.60 μmol) was added, and the immediate and quantitative formation of the compound $\mathbf{10}^{8+}$ was confirmed by ^{1}H NMR analysis of the reaction mixture. A saturated aqueous solution containing NH_4PF_6 was added and MeCN was removed under reduced pressure. The resultant precipitate was collected by filtration, washed with H_2O, and dried in *vacuo* to give the compound **10**•8PF_6 (7.12 mg) as a dark green solid. ^{1}H NMR (500 MHz, CD_3CN, 298 K): δ 9.30 (d, $^3J_{HH}$ = 6.0 Hz, 4H, H_α), 9.26 (d, $^3J_{HH}$ = 7.3 Hz, 4H, $H'_{\alpha+}$ (CH_2)), 9.14 (d, $^3J_{HH}$ = 6.5 Hz, 4H, H'_α (Pd)), 8.71 (d, $^3J_{HH}$ = 6.4 Hz, 4H, $H_{\alpha+}$ (CH_2)), 7.89 (d, $^3J_{HH}$ = 7.2 Hz, 4H, $H'_{\beta+}$ (CH_2)), 7.76 (d, $^3J_{HH}$ = 6.9 Hz, 4H, H_β (Pd)), 7.59 (d, $^3J_{HH}$ = 8.4 Hz, 2H, $H_{4/8}$ (DNP)), 7.57 (br m, 4H, H'_β (Pd)), 7.53 (d, $^3J_{HH}$ = 7.0 Hz, 4H, $H_{\beta+}$ (CH_2)), 7.51 (d, $^3J_{HH}$ = 8.4 Hz, 2H, $H'_{4/8}$ (DNP)), 7.48 (t, $^3J_{HH}$ = 8.1 Hz, 2H, $H_{3/7}$ (DNP)), 7.33 (d, $^2J_{HH}$ = 14.4 Hz, 2H, H_a), 7.27 (t, $^3J_{HH}$ = 8.0 Hz, 2H, $H'_{3/7}$ (DNP)), 7.07 (d, $^3J_{HH}$ = 7.6 Hz, 2H, $H_{2/6}$ (DNP)), 6.84 (d, $^2J_{HH}$ = 14.5 Hz, 2H, $H_{a'}$), 6.53 (d, $^3J_{HH}$ = 7.7 Hz, 2H, $H'_{2/6}$ (DNP)), 5.95 (s, 4H, H_{TTF}), 5.22 (br m, 2H, –CH_2NH_2), 4.82–4.72 (m, 4H, –OCH_2CH_2–), 4.64–4.44 (m, 6H, –CH_2NH_2), 4.32 (m, 2H, –OCH_2CH_2–), 4.16–4.13 (m, 6H, –OCH_2CH_2–), 4.08–3.55 (m, 34H, –OCH_2CH_2–), 3.48 (m, 2H, –OCH_2CH_2–), 3.39 (m, 2H, –OCH_2CH_2–), 3.02–2.84 (m, 12H, –CH_2NH_2 / –OCH_2CH_2–); ^{13}C NMR (125 MHz, CD_3CN, 298 K): δ 155.0 (C), 155.0 (CH), 154.4 (C), 153.7 (CH), 152.6 (C), 151.3 (C), 145.5 (CH), 144.6 (CH), 142.9 (C), 141.0 (C), 134.4 (C), 131.5 (C), 127.7 (CH), 127.4 (CH), 126.6 (C), 126.2 (CH), 125.8 (C), 125.6 (CH), 124.9 (CH), 124.7 (CH), 123.2 (C), 120.6 (C), 120.4 (CH), 119.2 (CH), 115.2 (CH), 114.1 (CH), 110.9 (C), 108.3 (C), 107.9 (CH), 106.6 (CH), 78.8 (CH_2), 73.2 (CH_2), 72.7 (CH_2), 71.7 (CH_2), 71.5 (CH_2), 71.5 (CH_2), 71.3 (CH_2), 71.2 (CH_2), 70.9 (CH_2), 70.9 (CH_2), 70.6 (CH_2), 70.0 (CH_2), 69.8 (CH_2), 69.3 (CH_2), 69.2 (CH_2), 68.7 (CH_2), 68.7 (CH_2), 48.1 (CH_2), 48.0 (CH_2); HR MS (ESI–TOF) Calcd for $C_{114}H_{140}N_{12}O_{20}Pd_2S_8P_8F_{48}$ (PF_6^- salt): m/z = 1668.2009 ($[M - 2(PF_6)]^{2+}$), 1063.8123 ($[M - 3(PF_6)]^{3+}$), 761.6181 ($[M - 4(PF_6)]^{4+}$), 508.3015 ($[M - 5(PF_6)]^{5+}$), 459.4238 ($[M - 6(PF_6)]^{6+}$); Found: m/z = 1668.2009 ($[M - 2(PF_6)]^{2+}$), 1063.8111 ($[M - 3(PF_6)]^{3+}$), 761.6169 ($[M - 4(PF_6)]^{4+}$), 508.3004 ($[M - 5(PF_6)]^{5+}$), 459.4225 ($[M - 6(PF_6)]^{6+}$).

2) [3]Catenane

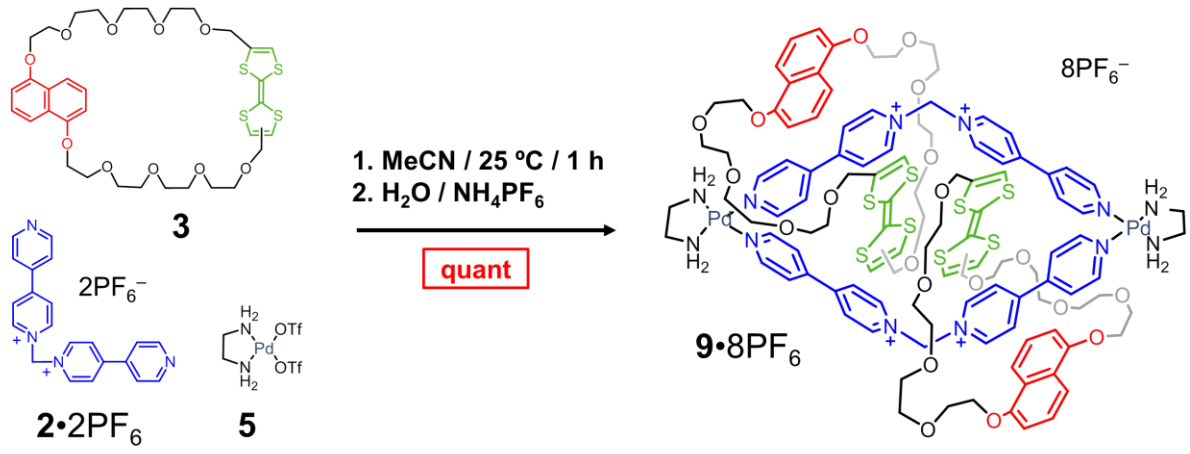
2.1) Pt(II) Complex **6**•8PF_6



Scheme S3. Synthesis of ***6•8PF₆***.

6•8PF_6: Ligand **2**·2PF_6 (10.7 mg, 17.4 μmol) was added to a solution of the crown ether **3** (12.0 mg, 16.2 μmol) dissolved in MeCN (840μL), and stirred for 1 h at ambient temperature. A 50 mM MeCN solution of ethylenediamineplatinum(II) bis(trifluoromethanesulfonate) **1** (418 μL, 20.9 μmol) was added to the mixture and the solution was stirred at 50 °C for 7 days. The crude mixture was subjected to preparative TLC (SiO_2, 1.0% NH_4PF_6 in Me_2CO), and dissolved in MeCN. A saturated aqueous solution containing NH_4PF_6 was added and MeCN was removed under reduced pressure. The resultant precipitate was collected by filtration, washed with H_2O, and dried in *vacuo* to give the compound **6**•8PF_6 (12.9 mg, 3.40 μmol) as a dark green solid in 39% yield. ^{1}H NMR (500 MHz, CD_3CN, 230 K) δ 9.44 (d, J = 6.1 Hz, 1.4H, H_α), 9.22 (d, J = 6.2 Hz, 0.6H), 9.17 (s, 1.8H), 9.11 (d, J = 6.4 Hz, 4.4H, $H'_{\alpha+}$ / H_α (CH_2 / Pt)), 9.02 (d, J = 5.6 Hz, 1.2H), 8.92 (d, J = 6.1 Hz, 1.4H), 8.76 (d, J = 6.2 Hz, 0.6H), 8.74 (d, J = 6.4 Hz, 1.4H, $H_{\alpha+}$ (CH_2)), 8.59 (d, J = 6.5 Hz, 0.6H), 8.39 (d, J = 6.4 Hz, 1.2H), 8.31 (d, J = 6.6 Hz, 2.8H, $H'_{\beta+}$ (CH_2)), 8.02 (br s, 1.4H), 7.92 (d, J = 6.3 Hz, 1H), 7.84 (d, J = 7.1 Hz, 2H, H'_β (Pt)), 7.47 – 7.34 (m, 6.4H, $H_{4/8}$ / $H_{3/7}$ / $H'_{4/8}$ (DNP)), 7.32 (m, 1.5 H, H_a), 7.24 (m, 2.7 H, $H'_{3/7}$ (DNP)), 7.12 (d, J = 6.2 Hz, 2.1 H, H_β (Pt)), 6.98 (d, J = 7.3 Hz, 0.6H), 6.95 (d, J = 7.4 Hz, 1.4H, $H_{2/6}$ (DNP)), 6.87 (d, J = 6.5 Hz, 0.6H), 6.84 – 6.74 (m, 5.3H, $H_{\beta+}$ / H'_a (CH_2)), 6.48 (d, J = 7.8 Hz, 1.4H, $H'_{2/6}$ (DNP)), 6.44 (d, J = 7.8 Hz, 0.6H), 5.91 (s, 1.4H), 5.86 (s, 1.4H), 5.85 (s, 2H), 5.75 (s, 0.6H), 4.97 (t, J = 10.9 Hz, 0.6H), 4.86 (m, 8.2H), 4.73 (t, J = 10.5 Hz, 2H), 4.28 – 3.40 (m, 65.5H), 2.74 (m, 7.8H), 2.55 (s, 0.6H). HR MS (ESI–TOF) Calcd for $C_{114}H_{140}N_{12}O_{20}Pt_2S_8P_8F_{48}$ (PF_6^- salt): m/z = 1757.2612 ($[M – 2(PF_6)]^{2+}$), 1123.1859 ($[M – 3(PF_6)]^{3+}$); Found: m/z = 1757.2570 ($[M – 2(PF_6)]^{2+}$), 1123.1866 ($[M – 3(PF_6)]^{3+}$).

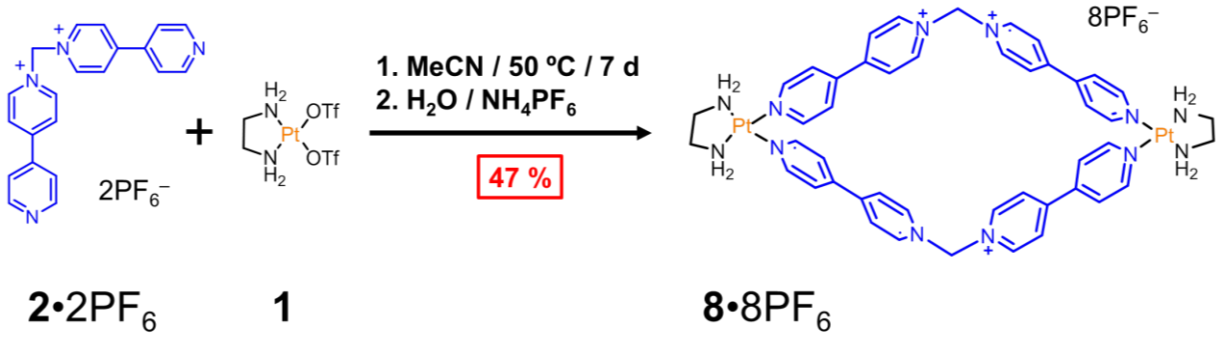
2.2) Pd(II) Complex **9**•8PF_6



Scheme S4. Synthesis of ***9•8PF$_6$***.

9•8PF$_6$: Ligand **2**·2PF_6 (2.50 mg, 4.00 μmol) was added to a solution of crown ether **4** (2.79 mg, 2.00 μmol) in MeCN (520 μL), and the mixture was stirred at ambient temperature for 1 h. A 50 mM MeCN solution of ethylenediaminepalladium(II) bis (trifluoromethanesulfonate) **5** (95 μL, 4.60 μmol) was added, and the immediate and quantitative formation of the compound $\mathbf{9}^{8+}$ was confirmed by ^{1}H NMR analysis of the reaction mixture. A saturated aqueous solution containing NH_4PF_6 was added and MeCN was removed under reduced pressure. The resultant precipitate was collected by filtration, washed with H_2O, and dried in *vacuo* to give the compound **9**•8PF_6 (6.98 mg) as a dark green solid. ^{1}H NMR (500 MHz, CD_3CN, 230 K) δ 9.52 (d, J = 5.9 Hz, 1H), 9.50 (d, J = 6.0 Hz, 2H), 9.32 (s, 2H), 9.20 (d, J = 6.7 Hz, 5H, H_α), 9.15 – 9.09 (m, 4H, H'$_\alpha$ / H'$_{\alpha+}$ (Pd / CH_2)), 9.04 (d, J = 6.0 Hz, 2H, H'$_\alpha$ / H'$_{\alpha+}$ (Pd / CH_2)), 9.01 (d, J = 6.1 Hz, 2H), 8.99 – 8.94 (m, 1H, $H_{\alpha+}$ (CH_2)), 8.85 (d, J = 6.4 Hz, 2H), 8.74 (d, J = 6.1 Hz, 2H), 8.60 (d, J = 6.3 Hz, 1H), 8.47 (d, J = 6.6 Hz, 2H, H_β), 8.35 (t, J = 6.6 Hz, 6H, H'$_\beta$ / $H_{\beta+}$ (Pd / CH_2)), 8.19 (d, J = 6.4 Hz, 2H), 8.04 – 7.99 (m, 2H), 7.93 – 7.89 (m, 5H, H'$_\beta$ (Pt)), 7.45 – 7.30 (m, 12H, $H_{4/8}$ / H'$_{4/8}$ / $H_{3/7}$), 7.30 – 7.23 (m, 4H, H_a), 7.18 (t, J = 8.0 Hz, 2H, H'$_{3/7}$), 7.16 – 7.10 (m, 3H), 6.96 (td, J = 6.9, 5.7, 3.2 Hz, 3H, $H_{2/6}$), 6.90 (dd, J = 6.6, 2.2 Hz, 1H, H'$_a$), 6.89 – 6.80 (m, 5H), 6.72 (dd, J = 6.9, 2.3 Hz, 1H), 6.69 (dd, J = 6.9, 2.2 Hz, 2H), 6.45 (d, J = 7.8 Hz, 2H, H'$_{2/6}$), 6.41 (d, J = 7.7 Hz, 1H), 5.90 (s, 2H, H_{TTF}), 5.87 (s, 1H), 5.25 – 5.40 (m, 3H, –CH_2NH_2), 5.11 – 4.69 (m, 6H, –OCH_2–), 4.66 – 4.31 (m, 10H, –CH_2NH_2), 4.27 – 3.34 (m, 58H). HR MS (ESI–TOF) Calcd for $C_{114}H_{140}N_{12}O_{20}Pd_2S_8P_8F_{48}$ (PF_6^- salt): m/z = 1668.7012 ([M – 2(PF_6)]$^{2+}$); Found: m/z = 1668.6996 ([M – 2(PF_6)]$^{2+}$).

3) Organoplatinum square



Scheme S5. Synthesis of ***8•8PF$_6$***.

8•8PF$_6$: The organoplatinum square was prepared according to slightly modified literature procedure.[S2] A 50 mM MeCN solution of **1** (845 μL, 42.2 μmol) was added to a solution of ligand **2**·2PF$_6$ (50.0 mg, 32.5 μmol) in MeCN (4.5 mL) and the mixture was stirred at 50 °C for 7 days. The resultant mixture was cooled down and treated with ether (40 ml). The precipitate was collected by filtration and a suspension of this material in H_2O (8 ml) was stirred at room temperature with Amberlite CG-400 (0.5 g) for 1 day. The resin was removed by filtration and a saturated aqueous solution containing NH_4PF_6 was added to the filtrate. The white precipitate was purified by preparative TLC (SiO_2, 1.0% NH_4PF_6 in Me_2CO), and dissolved in MeCN. The collected fraction in MeCN was concentrated *in vacuo* and treated with cold H_2O and an excess of NH_4PF_6 to precipitate a white solid that was collected by filtration and dried in *vacuo* to give the compound **8**•8PF$_6$ (17.7 mg, 47%). ^{1}H NMR (500 MHz, CD_3CN, 298 K): δ 9.05 (d, $^3J_{HH}$ = 6.9 Hz, 8H), 8.40 (d, $^3J_{HH}$ = 7.0 Hz, 8H), 7.91 (d, $^3J_{HH}$ = 6.8 Hz, 8H), 4.92 (br, 8H), 2.79 (br, 8H); ^{13}C NMR (125 MHz, CD_3CN, 298 K): δ 155.5 (C), 154.0 (CH), 146.6 (CH), 144.6 (C), 126.2 (CH), 78.5 (CH_2), 48.3 (CH_2).

B. NMR and MS Characterization

1) Molecular Solomon link

1.1) NMR Spectroscopic analysis

a) ^{1}H NMR Spectrum

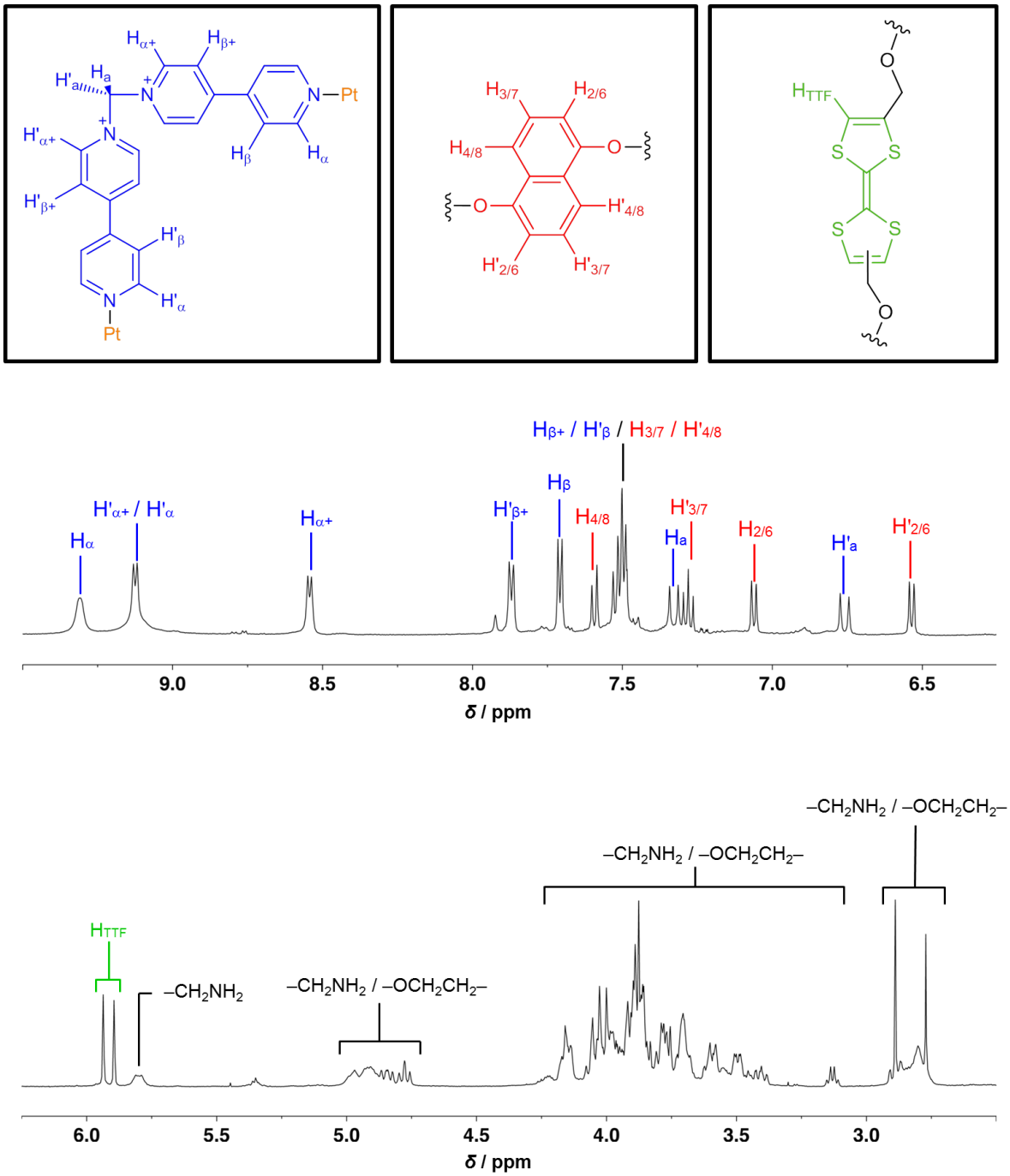


Figure S1. ^{1}H NMR spectrum (500 MHz, CD_3CN, 298 K) of **7**•8PF_6.

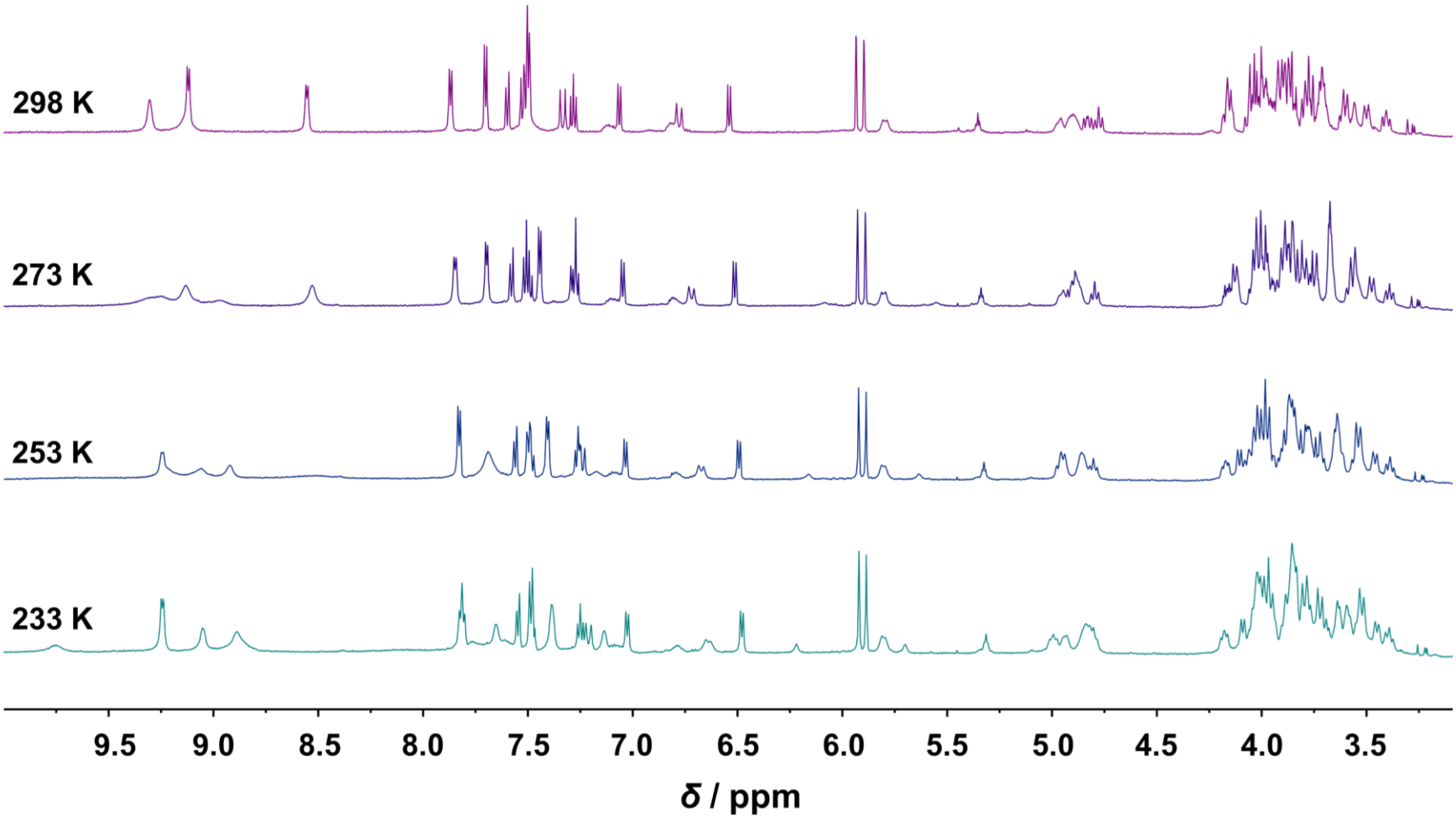


Figure S2. Variable temperature ^{1}H NMR spectra (600 MHz, CD_3CN) of **7**•8PF_6.

b) ^{1}H– ^{1}H COSY Spectrum

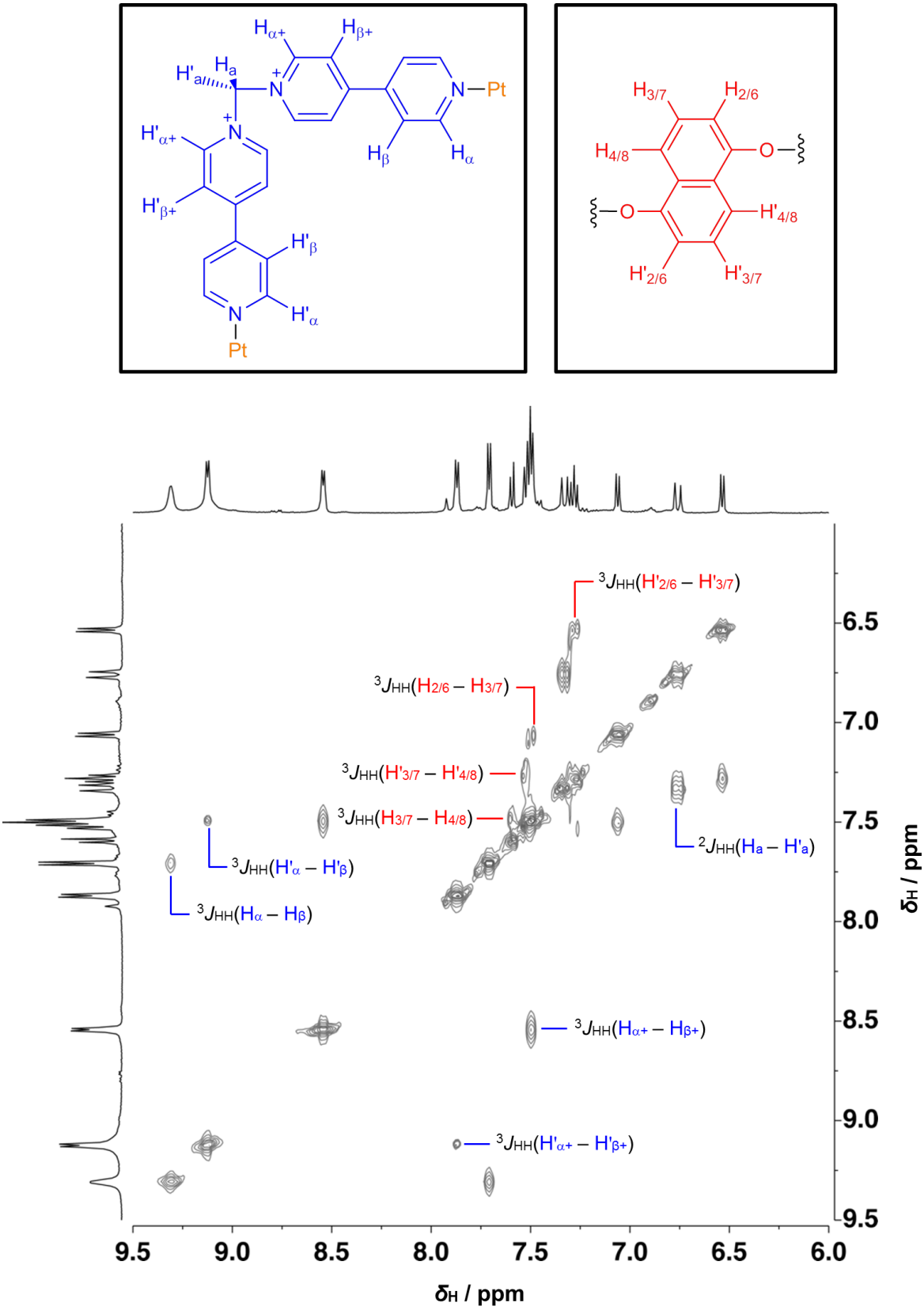


Figure S3. ^{1}H– ^{1}H COSY spectrum (expanded to 6.5–9.5 ppm, 500 MHz, CD_3CN, 298 K) of **7**•8PF_6.

c) ^{1}H DOSY NMR Spectrum

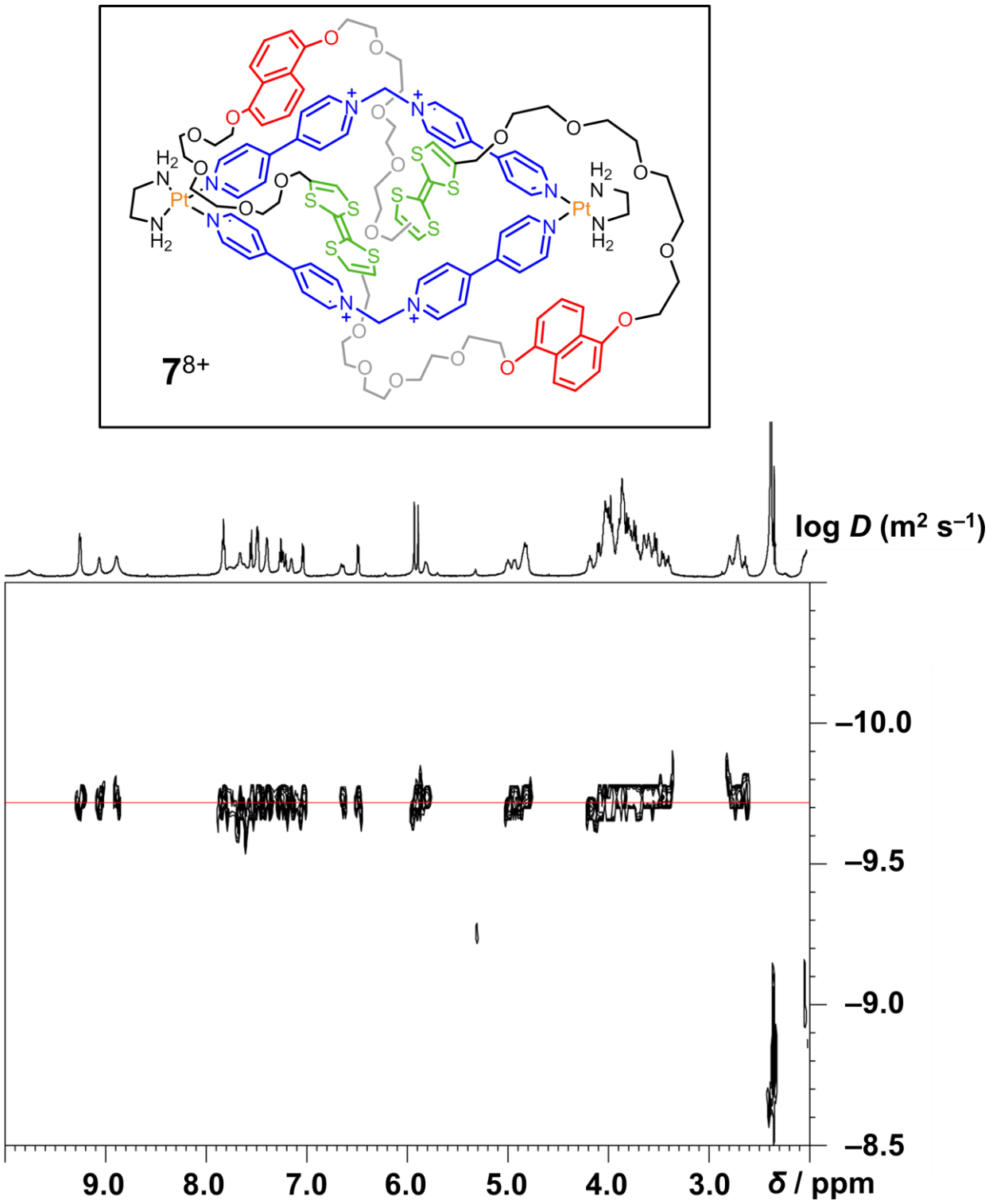


Figure S4. ^{1}H DOSY NMR spectrum (600 MHz, CD_3CN, 233 K) of **7**•8PF_6.

d) ^{13}C NMR Spectrum

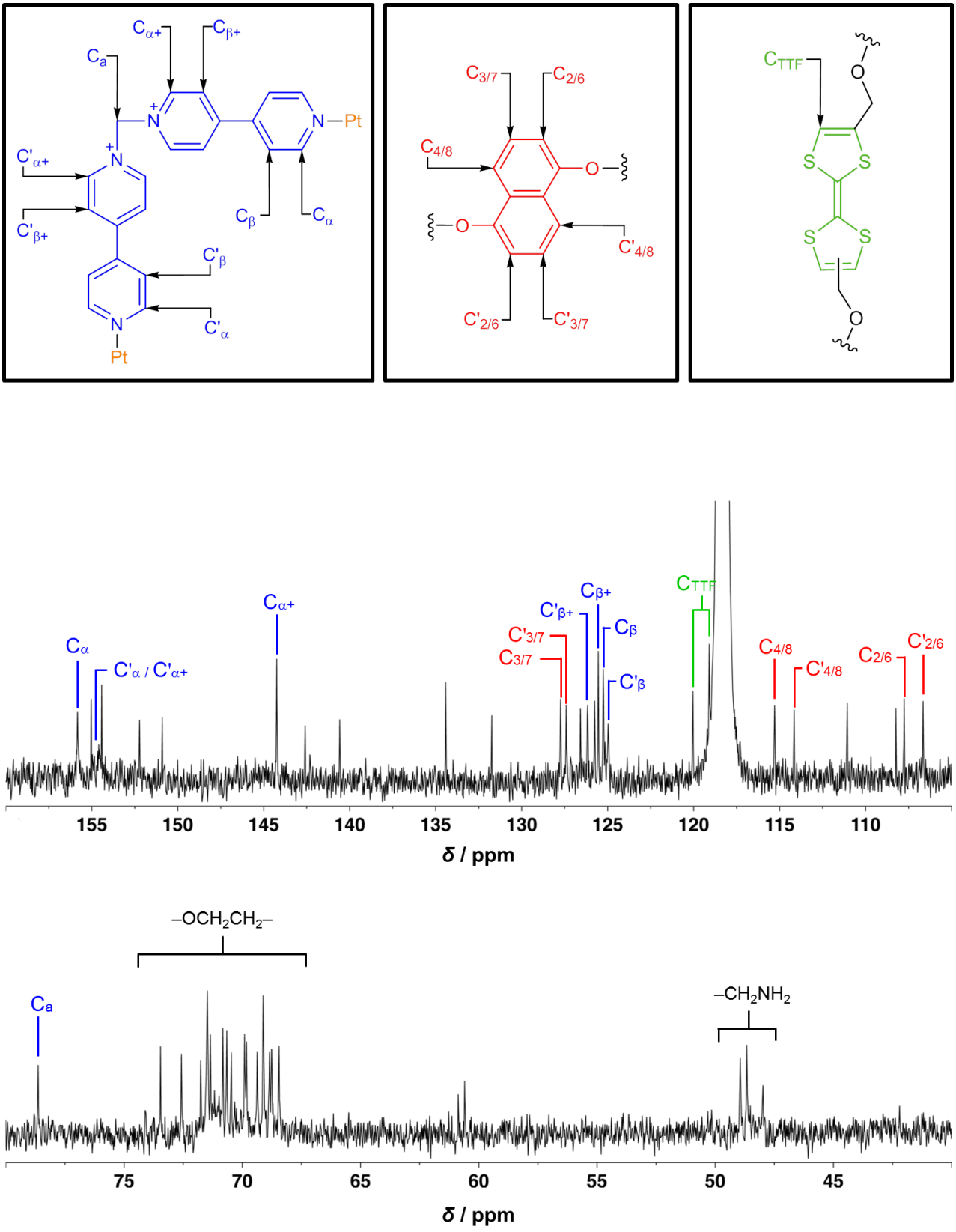


Figure S5. ^{13}C NMR spectrum (125 MHz, CD_3CN, 298 K) of **7**•8PF_6.

e) ^{1}H– ^{13}C HSQC Spectrum

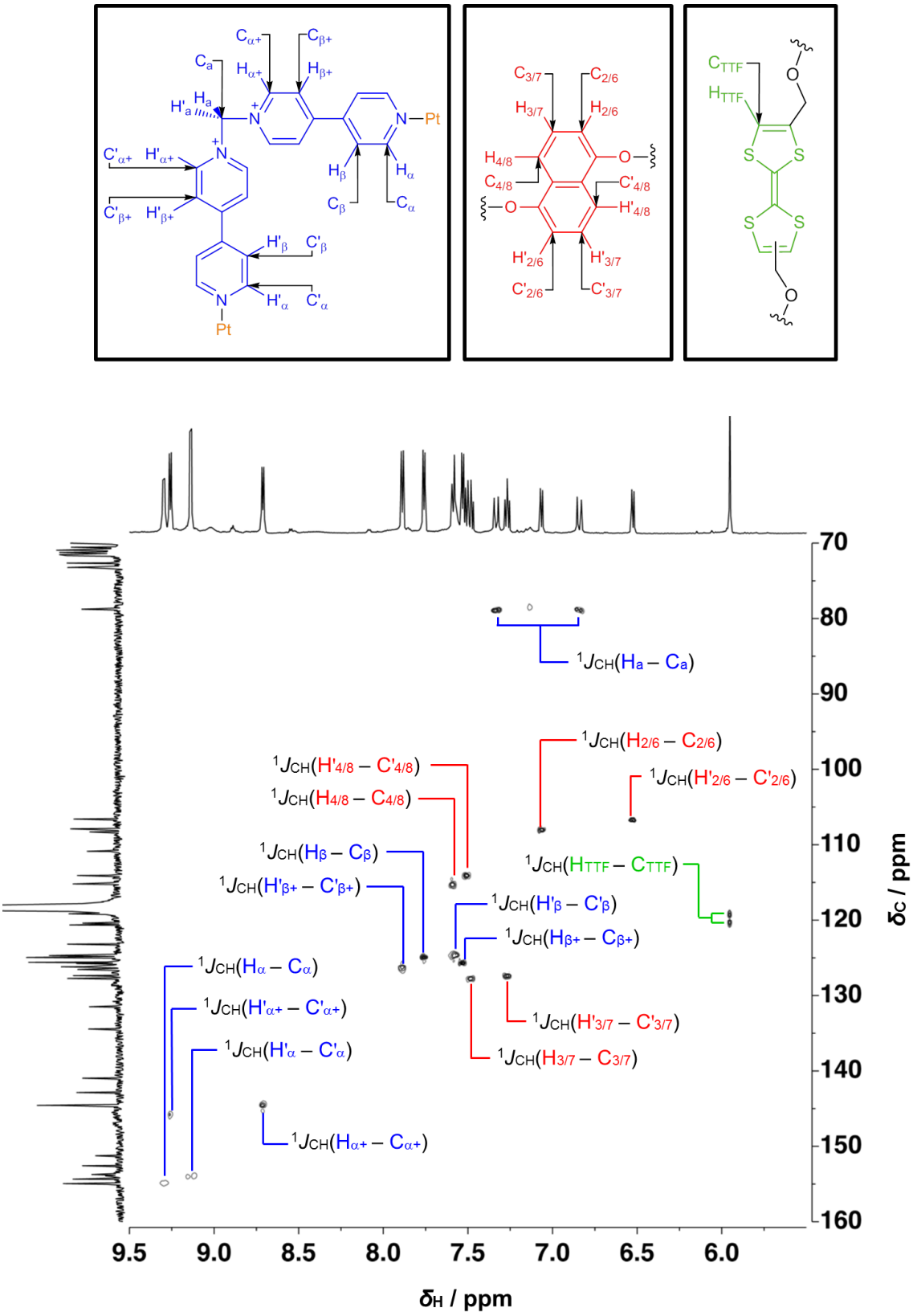


Figure S6. ^{1}H– ^{13}C HSQC spectrum (expanded to 6.5–9.5 ppm for ^{1}H and 70–160 ppm for ^{13}C nuclei, respectively, 500 MHz, CD_3CN, 298 K) of **7**•8PF_6.

f) $^{1}H–^{13}C$ HMBC Spectrum

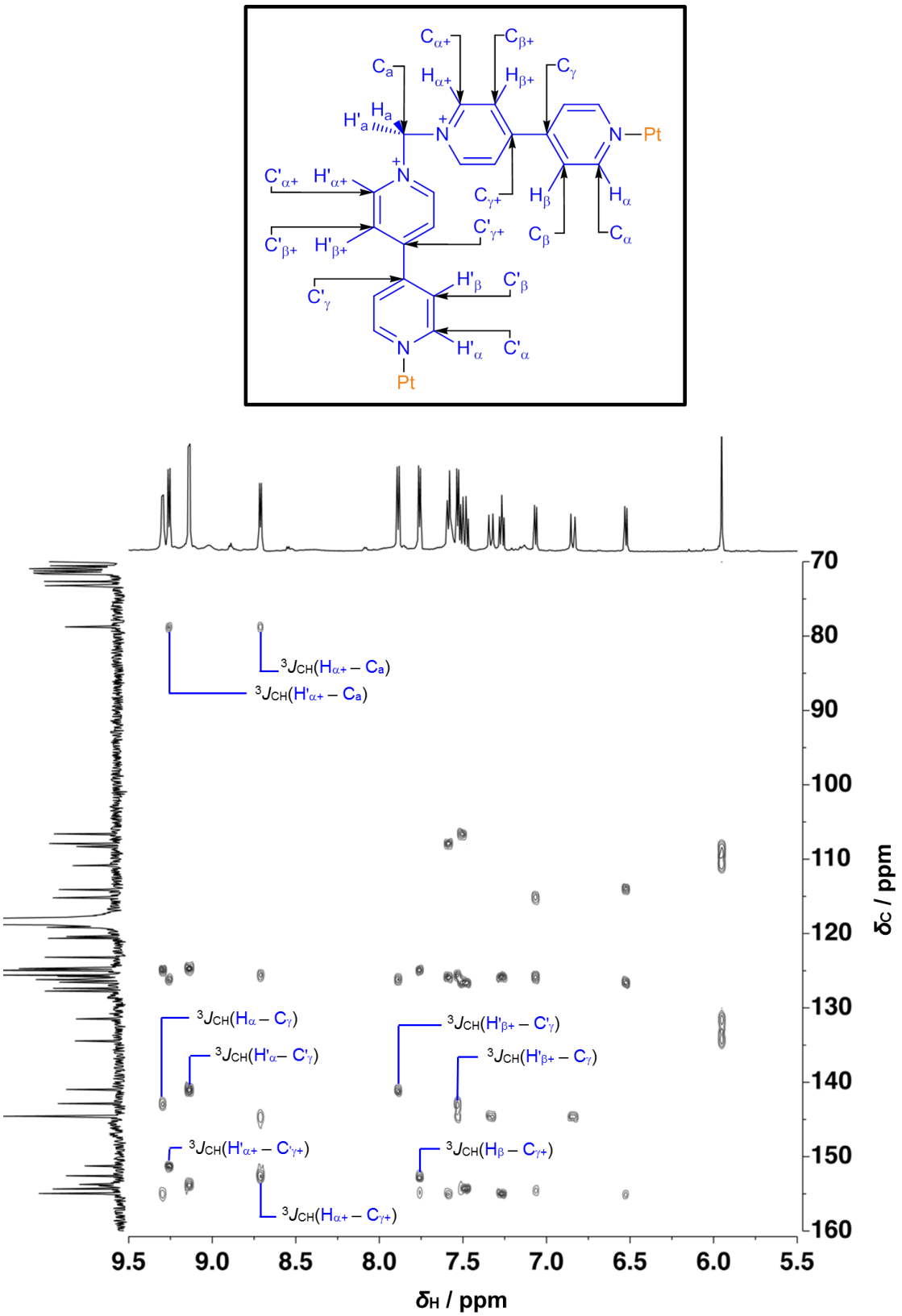


Figure S7. $^{1}H–^{13}C$ HMBC spectrum (expanded to 6.5–9.5 ppm for ^{1}H and 70–160 ppm for ^{13}C nuclei, respectively, 500 MHz, CD_3CN, 298 K) of **7**•8PF_6.

1.2) High-resolution mass spectrum (HRMS)

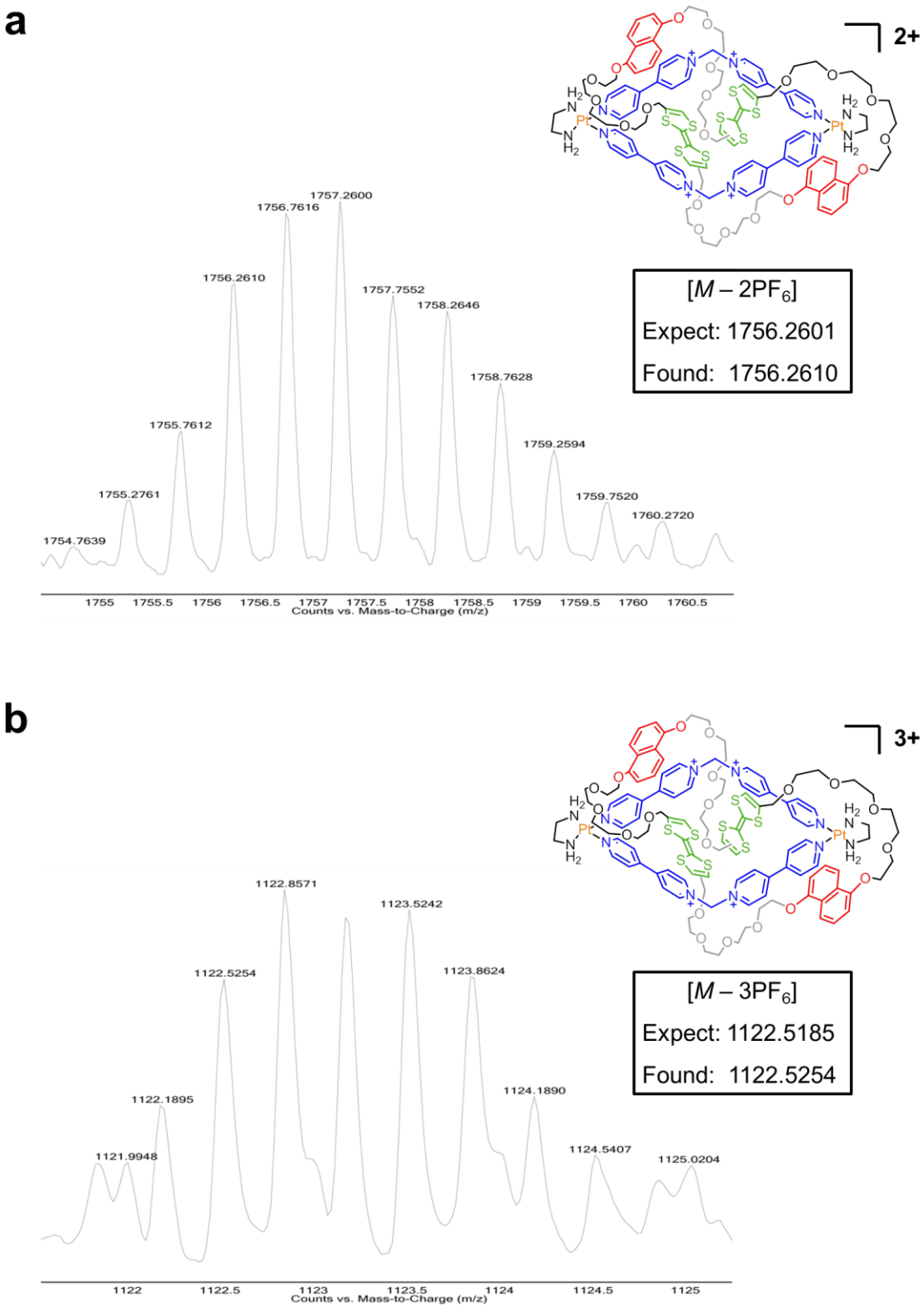


Figure S8. Expanded HRMS-ESI–API mass spectra of **7**·8PF_6: PF_6^- counterions losses associated with each charge state: (**a**) $[M - 2(PF_6)]^{3+}$, (**b**) $[M - 3(PF_6)]^{4+}$.

2) [3]Catenane

2.1) NMR Spectroscopic analysis

a) ^{1}H NMR Spectrum

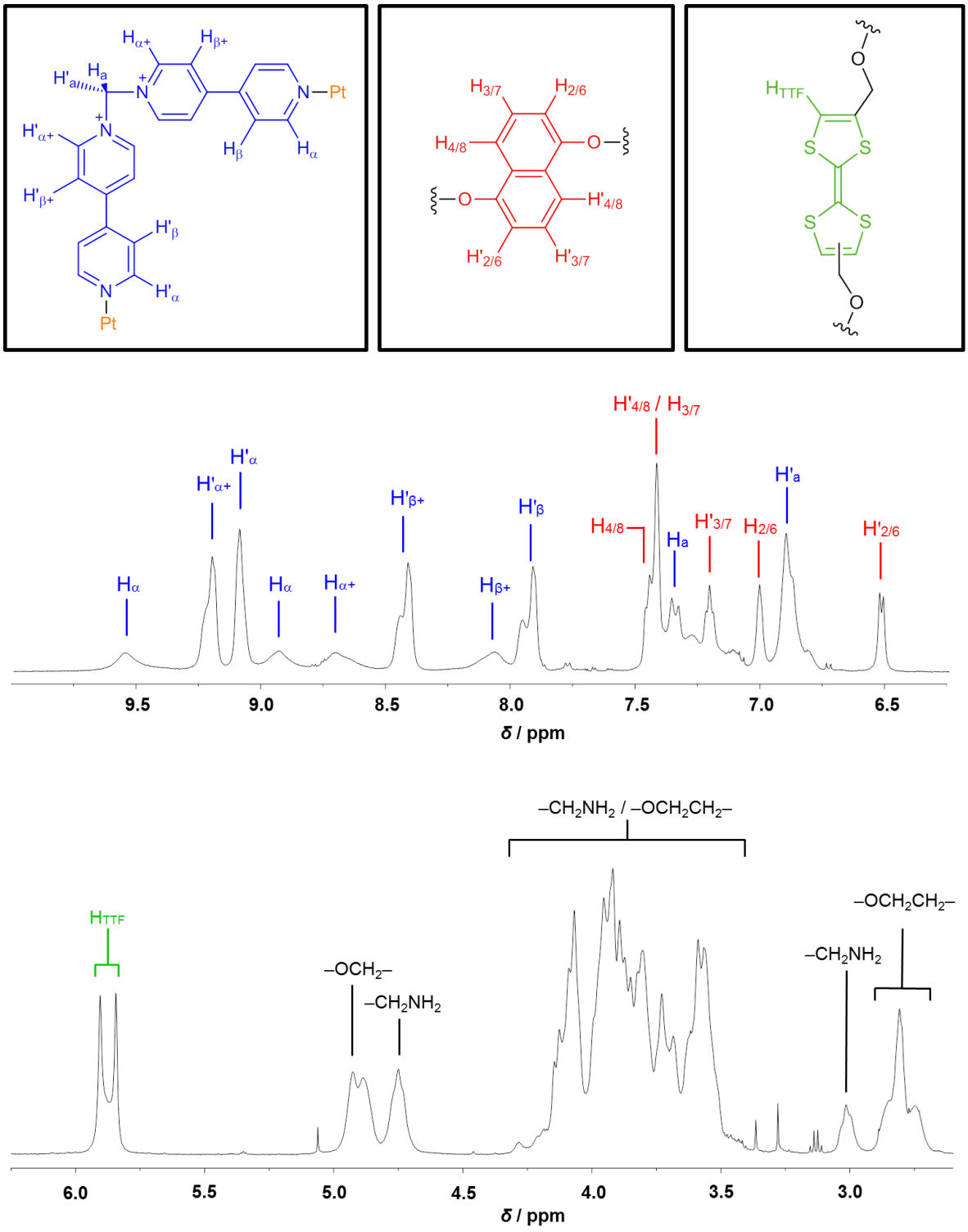


Figure S9. ^{1}H NMR spectrum (500 MHz, CD_3CN, 298 K) of **6**•8PF_6.

The ^{1}H NMR spectra of a CD_3CN solution of $\mathbf{6}^{8+}$ shows a significant line broadening at 298 K, which indicates the participation of the protons in rapid exchange processes on the ^{1}H NMR timescale. Variable temperature ^{1}H NMR spectra were employed (Figure S10) to evaluate the presence of this dynamic process.

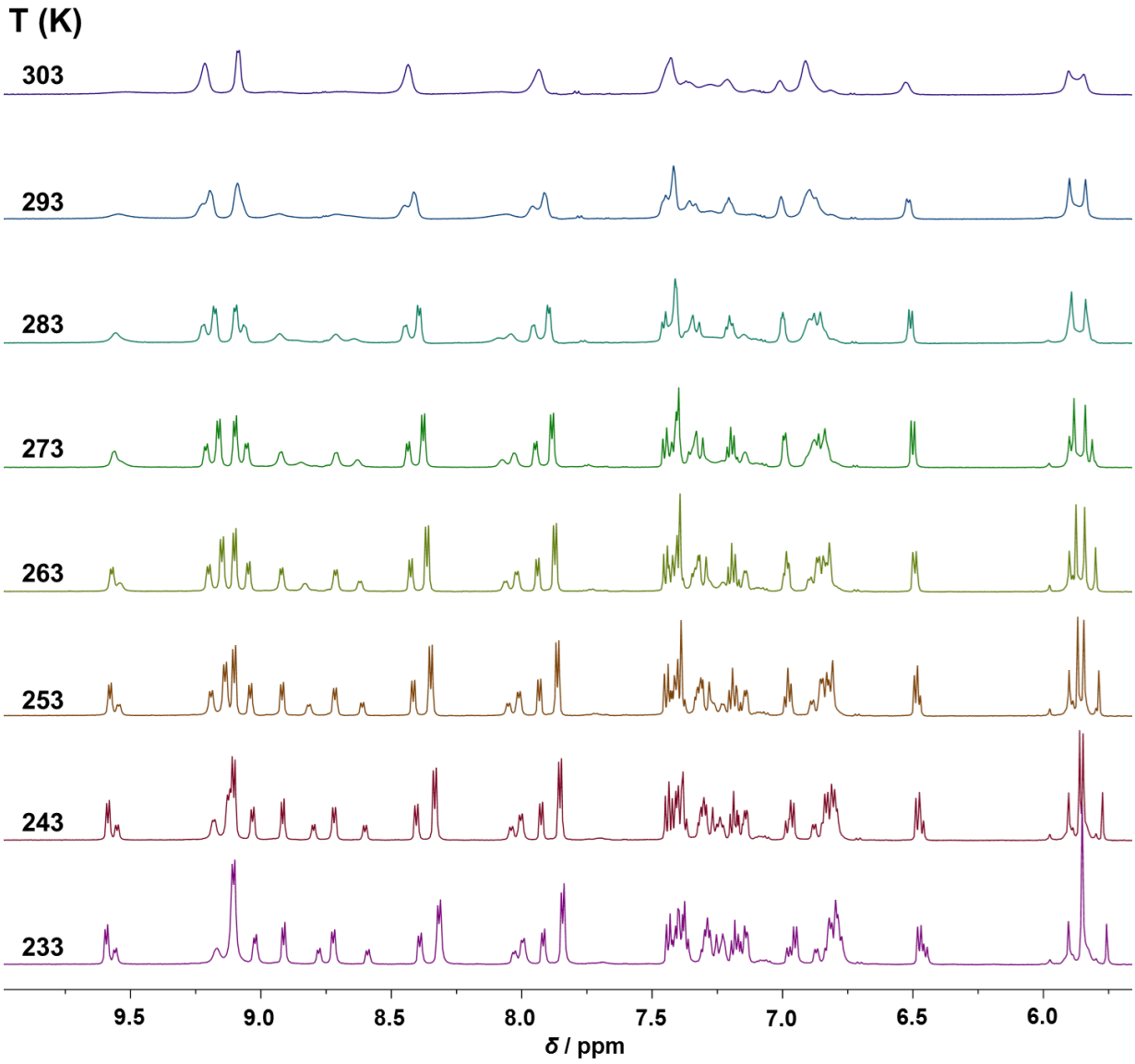


Figure S10. Variable temperature ^{1}H NMR spectra (600 MHz, CD_3CN) of **6**•$8PF_6$.

As the temperature is lowered and the exchange rates become slower on the ^{1}H NMR timescale the resonances separate into a set of distinct signals, pointing to the existence of dynamic processes within this [3]catenane.

b) ^{1}H– ^{1}H COSY Spectrum

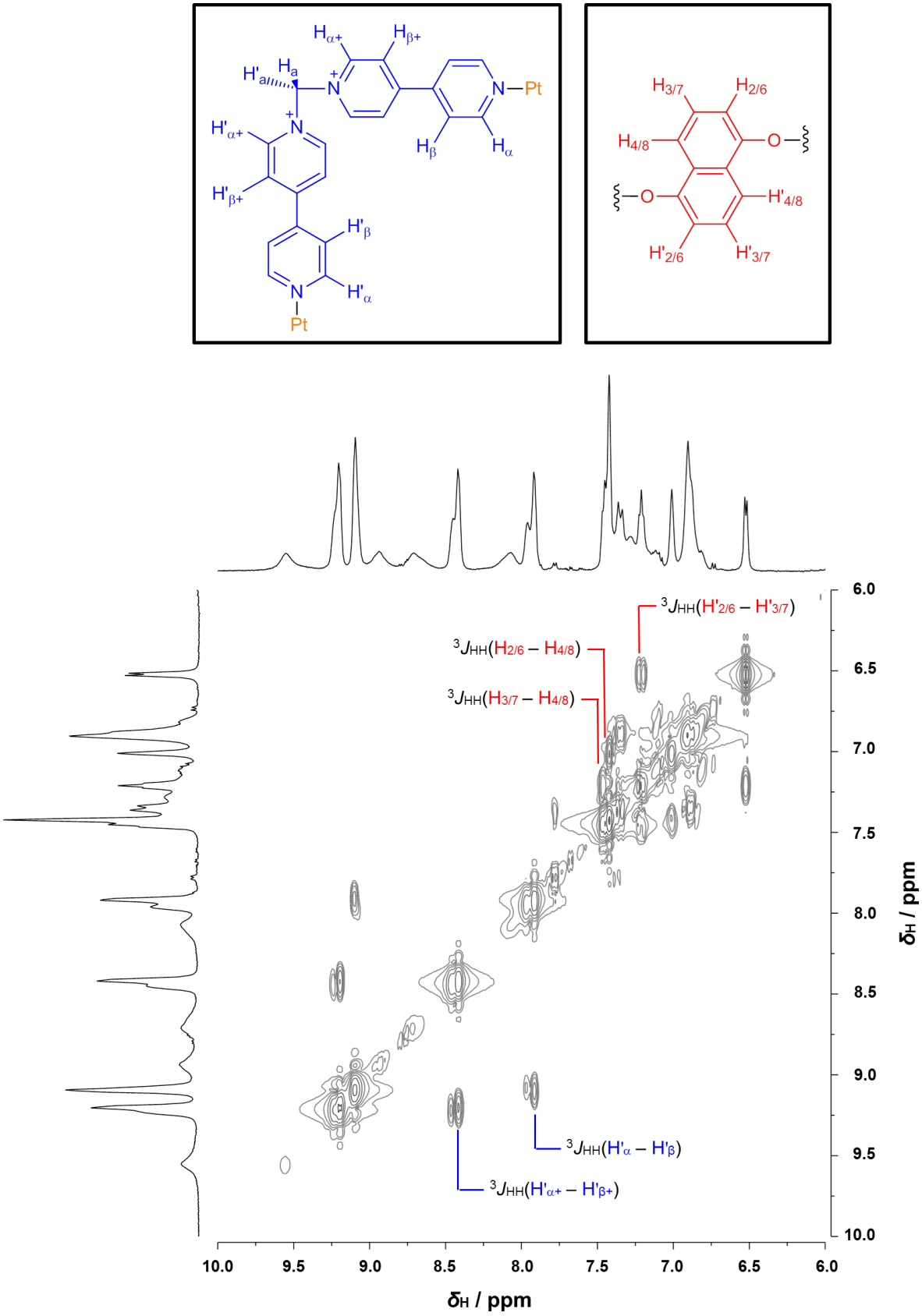


Figure S11. ^{1}H– ^{1}H COSY spectrum (expanded to 6.0–10.0 ppm, 500 MHz, CD_3CN, 298 K) of **6**•8PF_6.

c) $^{1}H–\ ^{1}H$ NOESY

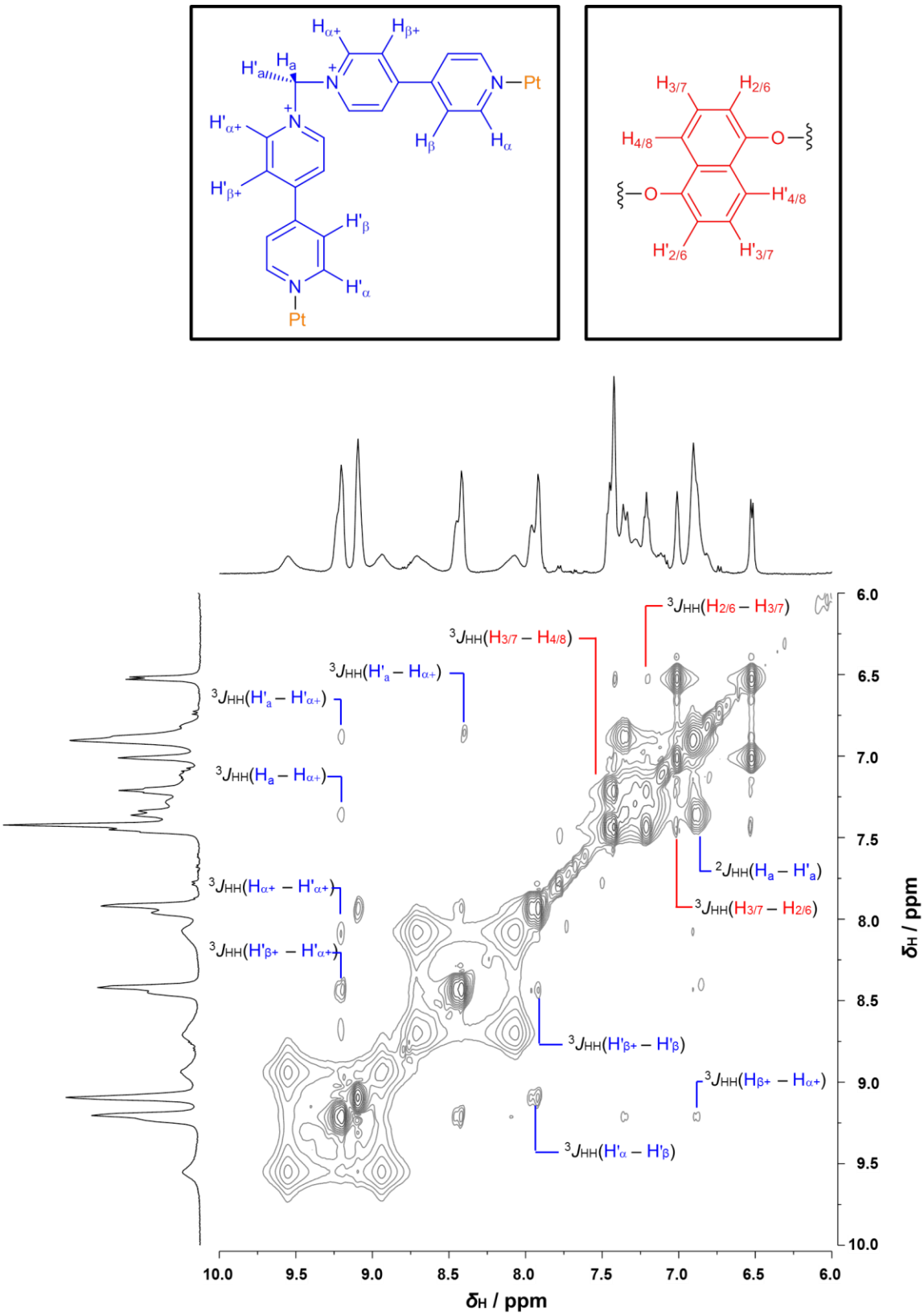


Figure S12. $^{1}H–\ ^{1}H$ NOESY spectrum (expanded to 6.0–10.0 ppm, 500 MHz, CD_3CN, 298 K) of **6**•8PF_6.

d) ^{1}H DOSY NMR Spectrum

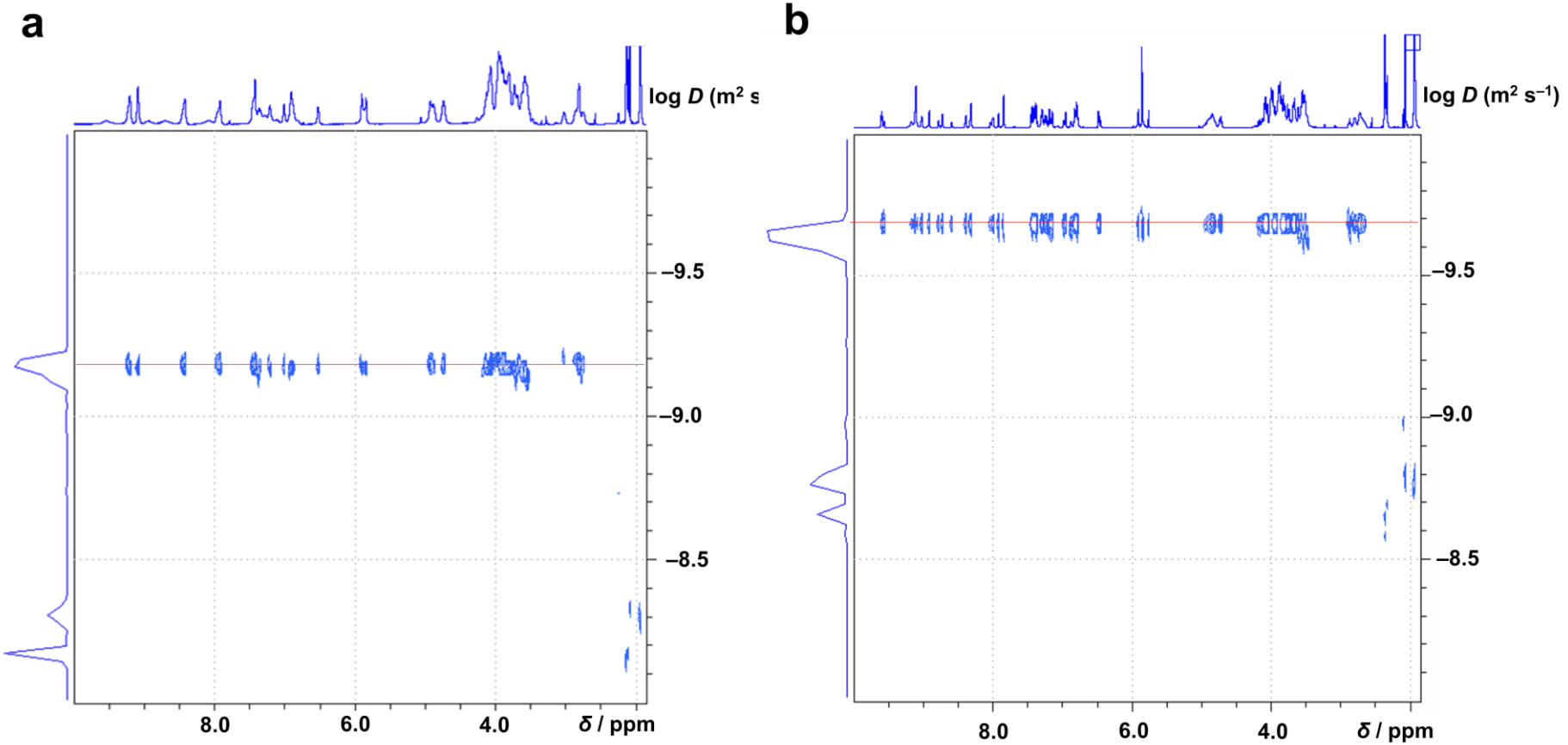


Figure S13. ^{1}H DOSY NMR spectrum (600 MHz, CD_3CN, 233 K) of **6**•8PF_6 at (**a**) 298 K and (**b**) 233 K.

e) ^{13}C NMR Spectrum

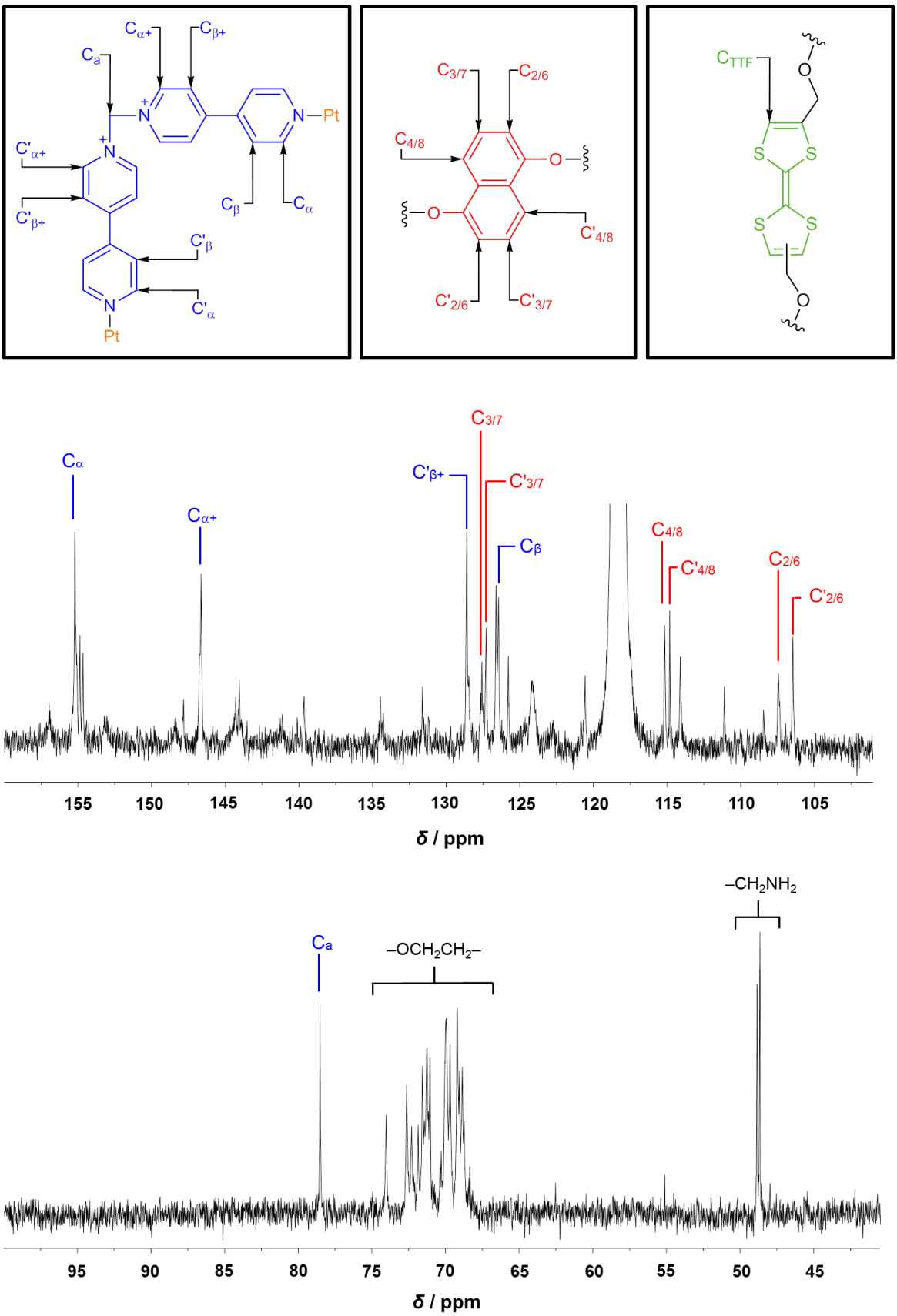


Figure S14. ^{13}C NMR spectrum (125 MHz, CD_3CN, 298 K) of **6**•8PF_6.

f) $^{1}H–\ ^{13}C$ HSQC Spectrum

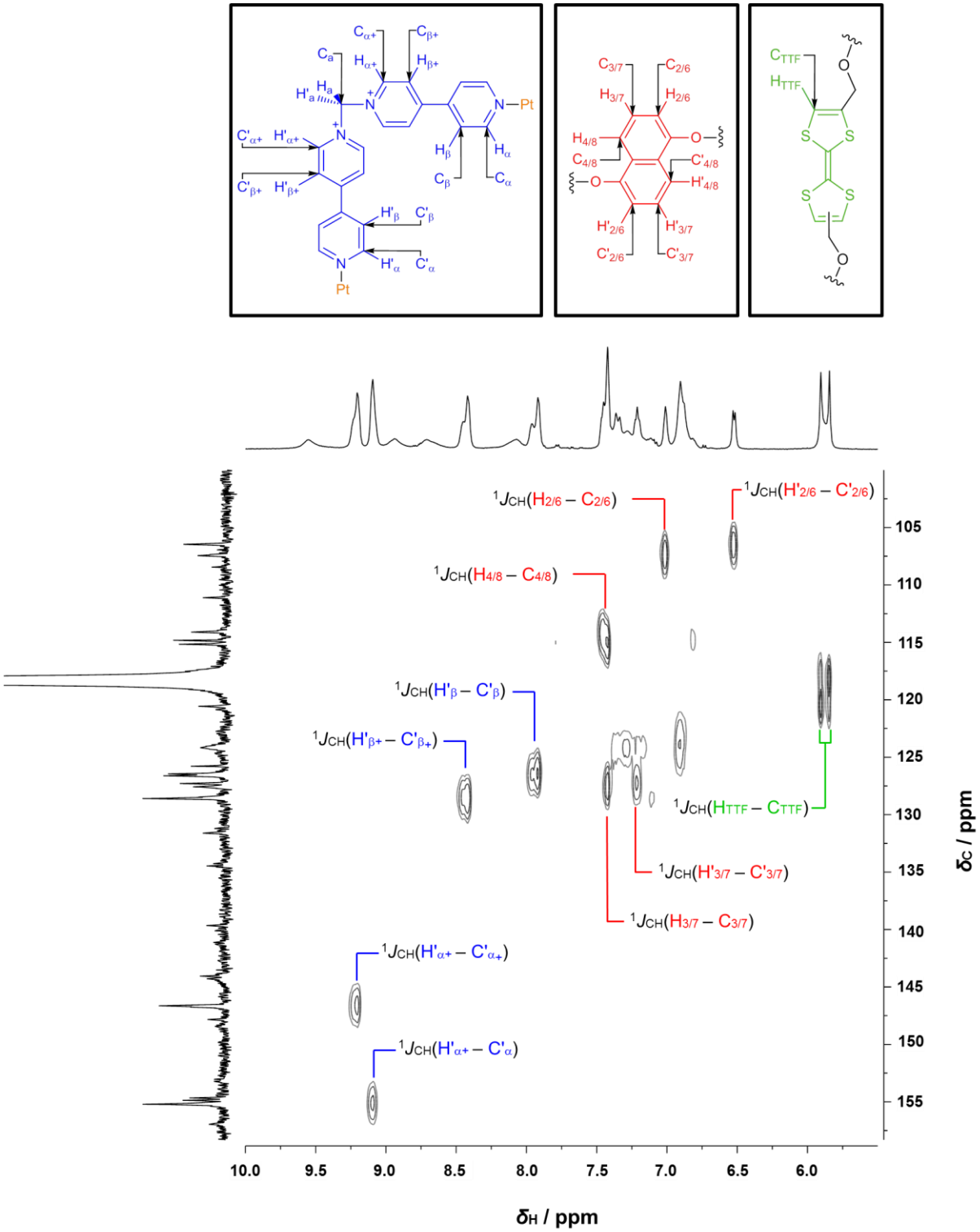


Figure S15. $^{1}H–\ ^{13}C$ HSQC spectrum (expanded to 6.0–10.0 ppm for ^{1}H and 100–160 ppm for ^{13}C nuclei, respectively, 500 MHz, CD_3CN, 298 K) of **6**•8PF_6.

2.2) High-resolution mass spectrum (HRMS)

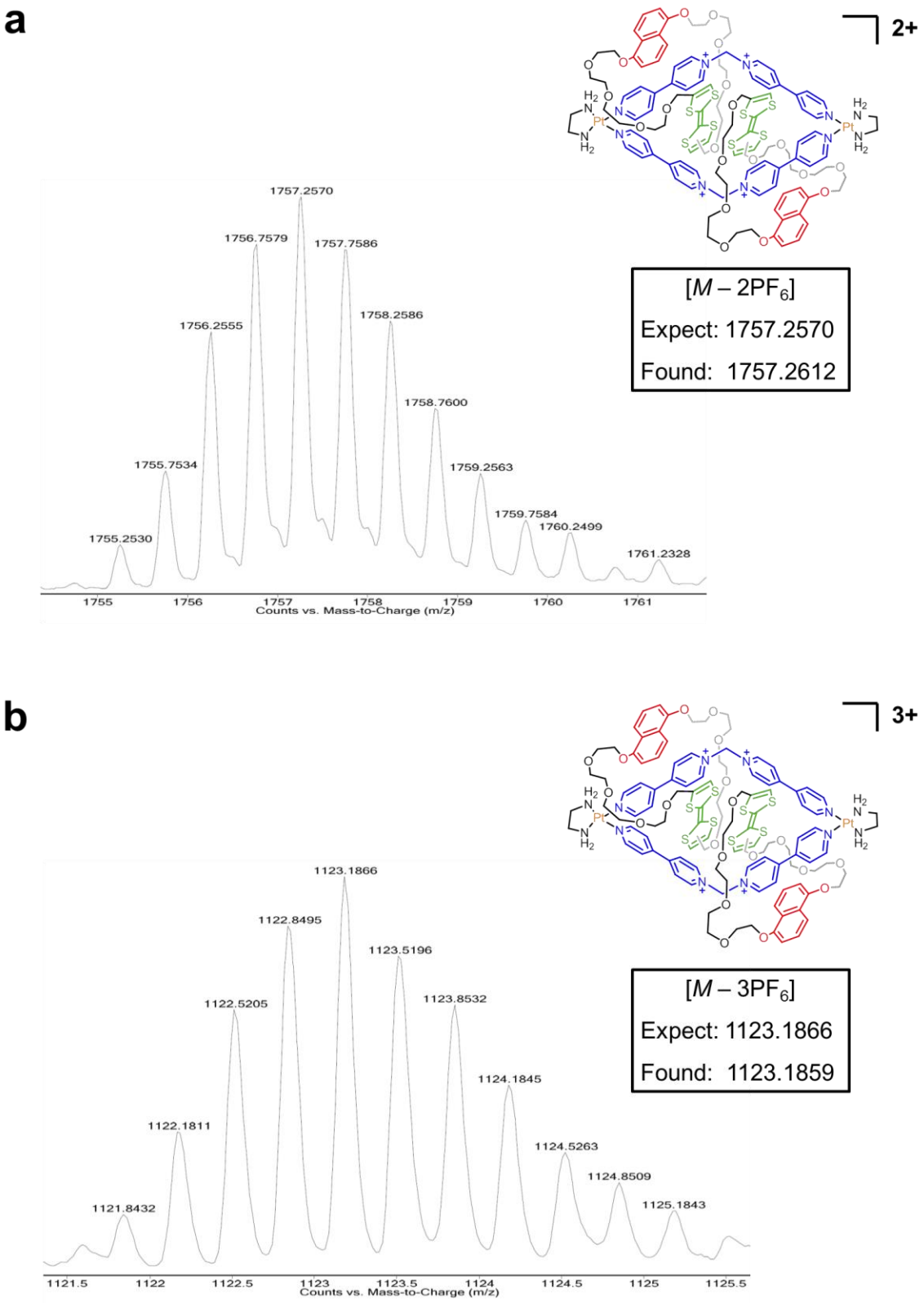


Figure S16. Expanded HRMS-ESI–API mass spectra of **6**•8PF_6: PF_6^- counterions losses associated with each charge state: (**a**) $[M - 2(PF_6)]^{3+}$, (**b**) $[M - 3(PF_6)]^{4+}$.

D. Crystallographic Characterizations

All crystallographic data has been deposited with the Cambridge Crystallographic Data Centre (CCDC) as supplementary publications, and are available free of charge via www.ccdc.cam.ac.uk/data_request/cif

1) Ring-in-ring complex (4⊂8) •8PF$_6$

1.1) Methods

Single crystals of **(4⊂8)**•8PF_6 were grown at 25 ºC by slow vapor diffusion of Et_2O into a MeCN solution containing an equivalent mixture of **4** and **8**•8PF_6 in equimolar mixture. The single crystals were mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa APEX CCD area detector, equipped with a CuKα microsource with MX optics.

1.2) Crystal data

$C_{114}H_{140}F_{48}N_{12}O_{20}P_8Pt_2S_8$, M = 3804.79, monoclinic, space group $C2/c$ (no. 15), a = 37.143(5), b = 13.161(3), c = 34.426(5) Å, β = 93.675(10)°, V = 16794(5) Å^3, T = 100.01 K, Z = 4, μ(CuKα) = 5.716. A total of 48795 reflections were collected, of which 14099 were unique (R_{int} = 0.0769). Final $wR(F_2)$ = 0.2244. CCDC number: 952941.

The solvent masking procedure as implemented in Olex2 was used to remove the electronic contribution of solvent molecules from the refinement.

1.3) Solid-state superstructure

The solid-state superstructure of **4**⊂**8**$^{8+}$ confirms (Figure S17) the existence in the solid-state of a ring-in-ring complex, in which two electron-rich TTF units are housed within the cavity of the organoplatinum square. The tetrathiafulvalene units form an acceptor–donor–donor–acceptor stack with the alongside electron-deficient $BIPY^+$ walls, revealing an average interplanar distance (Figure S8b) of 3.48 Å. Both TTF units of **4** located within the organoplatinum square exist in the *trans* configuration in the solid-state superstructure, a configuration that has been previously observed[S5] for TTF in different topologies.

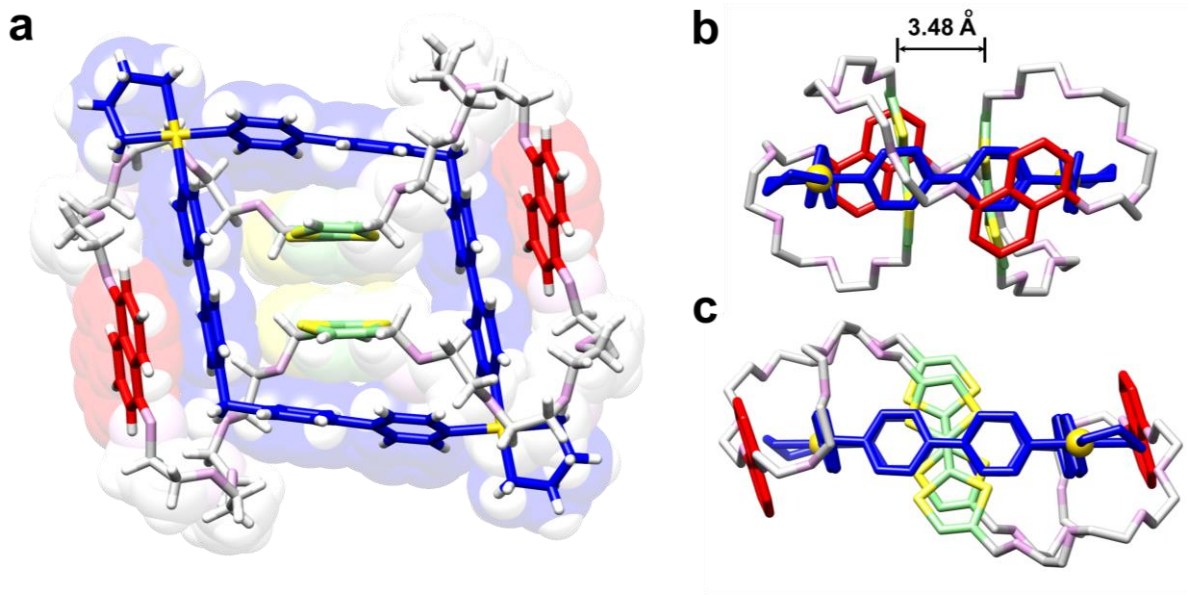


Figure S17. Solid-state superstructure of the ring-in-ring complex $\mathbf{4}\subset\mathbf{8}^{8+}$ between the crown ether **4** and the organoplatinum square $\mathbf{8}^{8+}$. Hydrogen atoms, MeCN solvent molecules and PF_6^- counterions are omitted for the sake of clarity. **a**, Combined space-filling and stick representation (plan-view) of the solid-state superstructure of the ring-in-ring complex. **b**, **c**, Stick representations of the single complex unit $\mathbf{4}\subset\mathbf{8}^{8+}$ displayed as two different side-on views, along with the average TTF interplanar spacing. The angle of offset is defined by the relative orientations of the C=C double bond in the TTF units. When the TTF units of **4** are housed in the organoplatinum square the angle of offset is 0º. The vertical offset, which is a measure of the offset between the planes of the TTF units, is close to 0.7 Å.

The DNP units take part in alongside short interplanar contacts (3.32 Å) with the outer faces of the $BIPY^+$ walls. The [π···π] stacking interactions are augmented by [C–H···O] interactions of the polyether loop which is folded onto the outer rim of the organoplatinum square.

2) Molecular Solomon link 7•8PF$_6$

2.1) Methods

Single crystals of **7**•8PF_6 were grown by slow vapor diffusion of *i*Pr_2O into a solution of the molecular Solomon link in MeCN at 25 ºC. The single crystals were bathed in inert oil and transfered to the cold gas stream of a Bruker APEX-II CCD diffractometer (CuKα radiation).

2.2) Crystal data

$C_{114}H_{140}F_{48}N_{12}O_{20}P_8Pt_2S_8 \bullet 13CH_3CN$, M = 4338.49, monoclinic, space group $P2_1/n$ (no. 14), a = 20.9976(11), b = 33.2264(17), c = 26.4897(15) Å, β = 100.672(3)°, V = 18161.5(17) Å^3, T =99.99 K, Z = 4, μ(CuKα) = 5.387 mm^{-1}. A total of 32608 reflections were collected, of which 32608 were unique. Final $wR(F_2)$ = 0.1454. CCDC number: 952939.

There was slight disorder in the carbon atoms of the glycol chains which were refined with distance restraints (SADI) for the C–C and C–O bonds.

2.3) Solid-state superstructure

The molecular Solomon link **7**·8PF_6 crystallizes as a racemic modification, as evidenced (Figure S18) by the enantiomeric pair of molecules present in the unit cell.

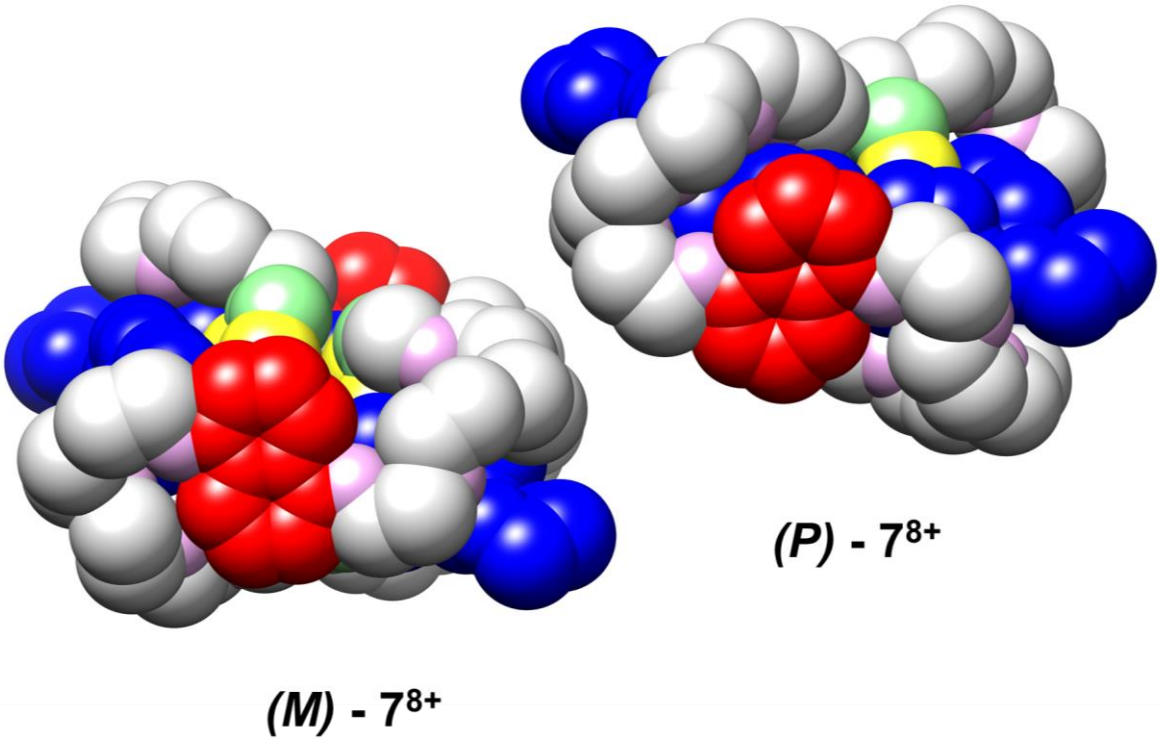


Figure S18. Space-filling representation of the centrosymmetrically related **(*M*)-7**$^{8+}$ and **(*P*)-7**$^{8+}$ enantiomers in the solid-state superstructure. The hydrogen atoms and counterions have been omitted for the sake of clarity.

With reference to their absolute chiralities, the molecules can be assigned the descriptor *P* or *M*, by using the screw-line system.[S4] As a consequence of the co-crystallization of equimolar amounts of *P* and *M* enantiomers, the crystal of the molecular Solomon link is optically inactive.

3) Oxidized molecular Solomon link 7•7PF$_6$•2ClO$_4$

3.1) Methods

The oxidized molecular Solomon link **7**•7PF$_6$•2ClO$_4$ was prepared by titration of 1.0 equiv of a solution of Fe(ClO$_4$)$_3$ in MeCN into a solution of **7**•8PF$_6$ in MeCN. The formation of mixed-valence state **7**$^{9+}$ in solution upon the addition of 1.0 equiv of Fe(ClO$_4$)$_3$ was monitored by UV-Vis-NIR spectroscopy.

Slow vapor diffusion of Et$_2$O into the MeCN solution containing **7**$^{9+}$ at 0 ºC during two weeks resulted in the separation of red plates of **7**•7PF$_6$•2ClO$_4$. The crystals were mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa APEX CCD area detector, equipped with a CuKα microsource with MX optics.

3.2) Crystal data

$C_{132}H_{167}Cl_2F_{42}N_{21}O_{28}P_7Pt_2S_8$, M = 4228.20, triclinic, space group $P\bar{1}$ (no. 2), a = 17.1706(8) , b = 20.6416(10), c = 27.7781(14) Å, α = 104.377(2), β = 102.420(2), γ = 99.953(2)°, V = 9043.6(8) Å^3, T = 99.99 K, Z = 2, μ(CuKα) = 5.556 mm^{-1}. A total of 179427 reflections were collected, of which 32487 were unique (R_{int} = 0.0324). Final $wR(F_2)$ = 0.1617. CCDC number: 952940.

The PF_6^- anions were subjected to various SADI restraints to preserve the octahedral environment around the P atoms. Chemically equivalent C–C, C–O, and 1,3-C···C distances in the disordered glycol chain, and C–C and C–N distances in disordered MeCN solvent molecules, were restrained to be equal (SADI). Global rigid bond (DELU) and similarity (SIMU) restraints were applied to keep displacement parameters reasonable.

The solvent masking procedure, as implemented in Olex2, was used to remove the electronic contribution of solvent molecules from the refinement. The formula reports only the atoms used in the refinement. Total solvent accessible volume/cell = 755.9 Å^3 [8.4%] and the total electron count/cell = 206.8.

3.3) Solid-state structure

The stability of the mixed-valence state of (TTF$_2$)$^{\bullet+}$ within the organoplatinum square makes it possible to investigate its solid-state structure by single crystal X-ray diffraction. The

presence of nine counterions, seven PF_6^- and two ClO_4^- counterions balances the charge on $\mathbf{7}^{9+}$ and is commensurate with an oxidation state of the molecular Solomon link in which one of the two tetrathiafulvalene units is in the radical-cationic state. It transpires that the structure of the mixed valence state of this molecular Solomon link crystallizes as a racemic modification of the *P* and *M* enantiomers. The space-filling representation of the centrosymmetrically related enantiomers is shown in Figure S19.

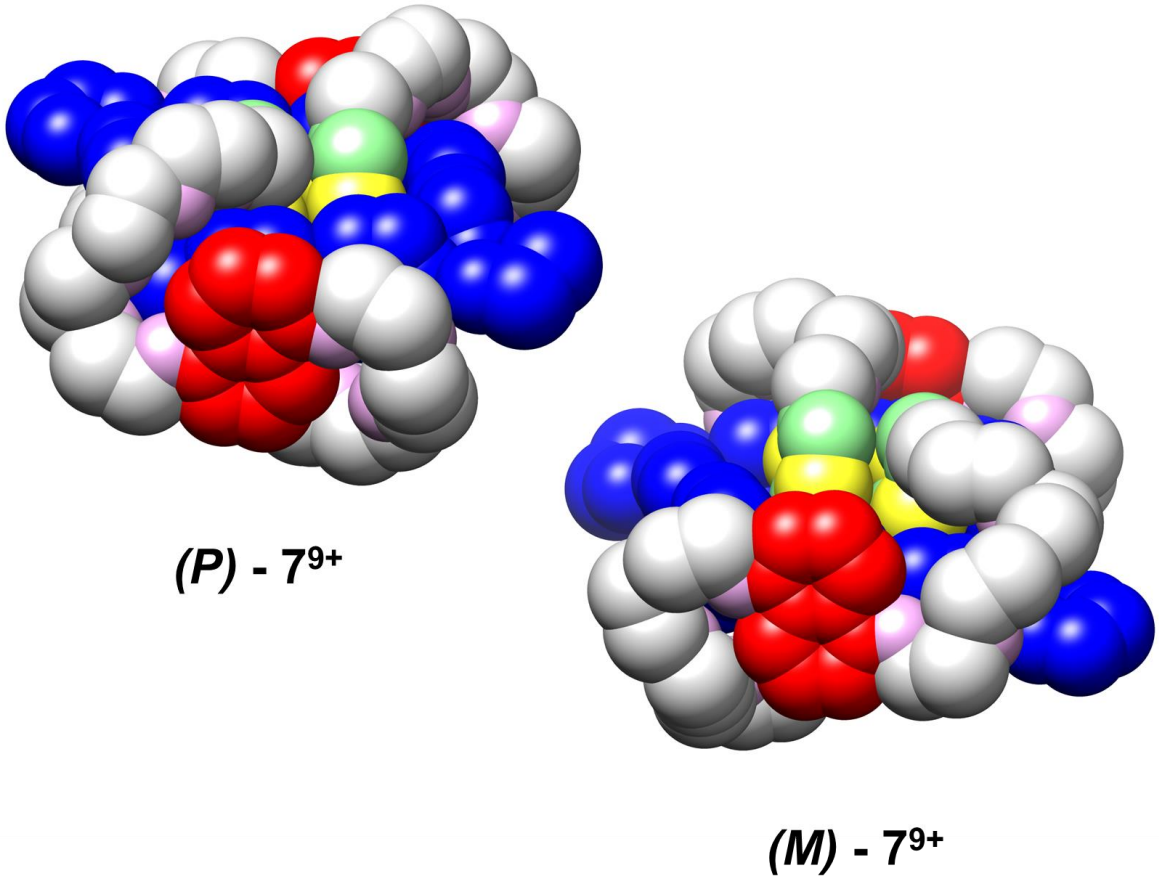


Figure S19. Space-filling representation of the centrosymmetrically related **(*M*)-$\mathbf{7}^{9+}$** and **(*P*)-$\mathbf{7}^{9+}$** enantiomers of the mixed-valence state of the molecular Solomon link in the solid-state superstructure. The hydrogen atoms and counterions have been omitted for the sake of clarity.

3.4) Counterions interaction with TTF units in the solid-state

The solid-state structure of the **7**•$7PF_6$•$2ClO_4$ was examined (Figure S20) to locate the presence of counterion-bridging interactions between the oxidized TTF units and the surrounding PF_6^- and ClO_4^- counterions. It has been shown[S6] that these type of interactions

occur during the oxidative dimerization of TTF units in order to overcome the repulsive Coloumbic force between $TTF^{\bullet+}$ radical cations.

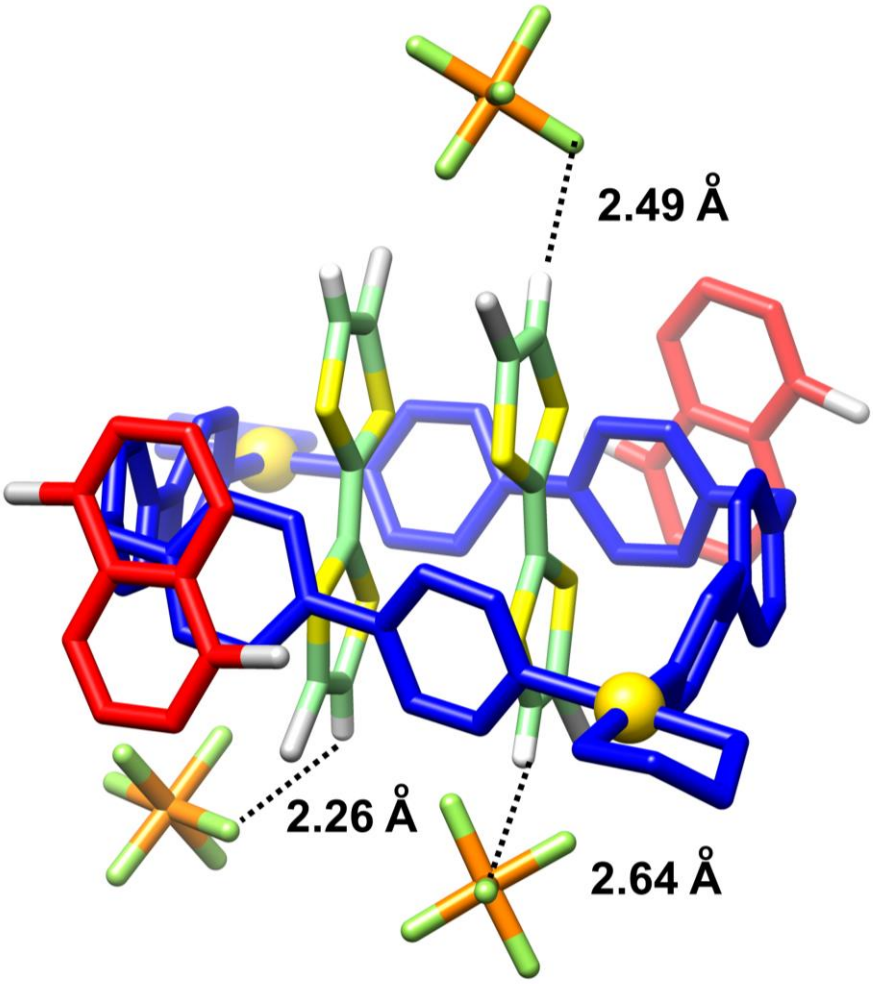


Figure S20. Stick representation of the short contacts between PF_6^- counterions and oxidized TTF units in the partial solid-state structure of **7**•7PF_6•2ClO_4. The close distances between the counterions and the TTF units within the organoplatinum square keep the charge species in close proximity. The polyether loop of the macrocycle, some counterions, the solvent molecules and non-TTF hydrogen atoms are omitted for clarity.

The presence of short [C−H···F] contacts has been observed for the hydrogen atoms of the TTF unit and fluorine atoms of the PF_6^- counterions. These close contacts contribute to the stabilization of the mixed-valence of TTF within the octacationic oraganoplatinum square despite the presence of Coulombic repulsions.

4) Molecular Solomon link 10•8PF$_6$

4.1) Methods

Single crystals of **10**•5PF$_6$•3OTf were grown by slow vapor diffusion of *i*Pr$_2$O into a solution of the molecular Solomon link in MeCN at 25 ºC. The single crystals were bathed in inert oil and transfered to the cold gas stream of a Bruker APEX-II CCD diffractometer (CuKα radiation).

4.2) Crystal data

$C_{114}H_{140}O_{20}S_8N_{12}Pd_2$•2.73$CF_3O_3S$•5.27$PF_6$•10$C_2H_3N$, M = 4049.14, triclinic, space group P-1 (no. 2), a = 15.7952(2), b = 20.6341(4), c = 29.3750(4) Å, α = 87.9230(10)°, β = 86.8350(10)°, γ = 76.4070(10)°, V = 9288.9(2) Å^3, T =99.99 K, Z = 2, μ(CuKα) = 4.065 mm^{-1}. A total of 209383 reflections were collected, of which 33341 were unique. Final $wR(F_2)$ = 0.2395. CCDC number: 975035.

The structure crystallized from a mixture of PF_6^- and OTf^- anions which are disordered in the cell. The solvent masking procedure as implemented in Olex2 was used to remove the electronic contribution of solvent molecules from the refinement. As the exact solvent content is not known, only the atoms used in the refinement model are reported in the formula here. Total solvent accessible volume/cell = 673.3 Å^3 [7.2%] Total electron count/cell = 139.7.

4.3) Solid-state structure

The solid-state structure of the molecular Solomon link **10**$^{8+}$ assembled under thermodynamic control using the pyridine-based ligand **2**·2PF$_6$ with ethylenediamine-chelated Pd(II) corner in the presence of the crown ether **4** shows (Figure S21) a molecular structure with C_2 symmetry. A stronger out-of-plane distortion was observed for the Pd(II) square when compared with the organoplatinum square. The average distance between the TTF units (ca. 3.63 Å) in the Pd(II) square complex is not dissimilar from that of the TTF units within the organoplatinum square of the molecular Solomon link **7**$^{8+}$, indicating that the TTF units do not interact with each other in the ground state. The less electron rich DNP moieties take part in alongside short interplanar contact with the outside faces of the bipyridinium walls (3.37 Å). The structure is also stabilized by [N–H···O] hydrogen bonds between the ethylenediamine hydrogens and the glycol oxygens (the average distance of N–O close contact pairs is 3.02 Å), as well as [C–H···O] close contacts observed between some of the glycol oxygens and the α-bipyridinium hydrogens.

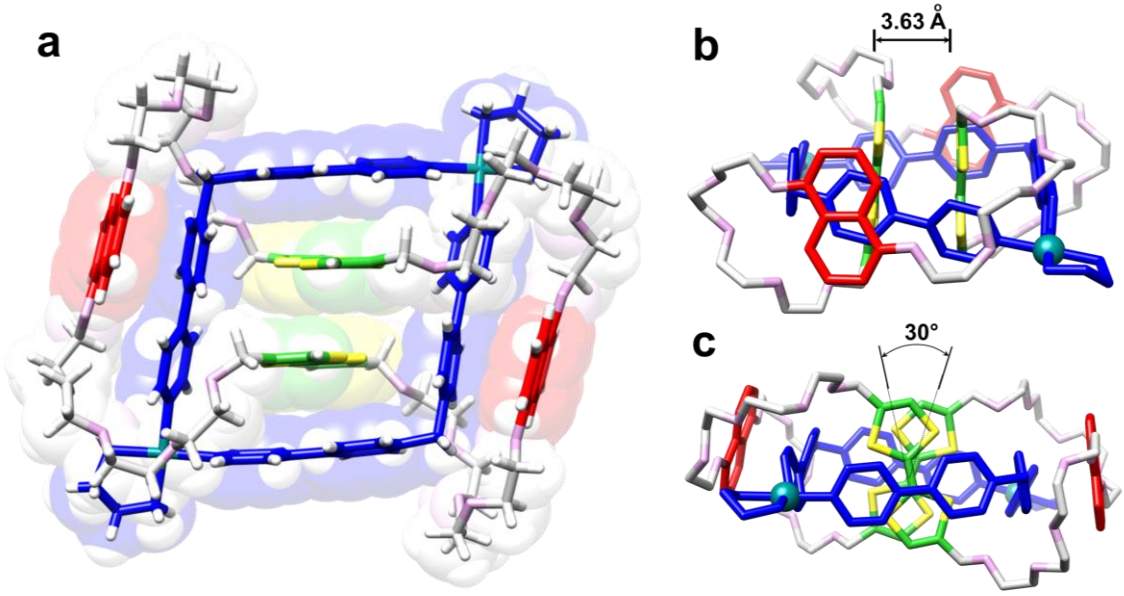


Figure S21. Solid-state structure of the molecular Solomon link $\mathbf{10}^{8+}$ based on Pd(II) metallocycle as (**a)** plan-view in a combined space-filling and stick representation and (**b,c**) two different side-on views in stick representation, along with the average TTF interplanar spacing and the angle of offset, defined by the relative orientations of the C-C double bonds in the TTF units. Only one enantiomer of the Solomon link, which has topological chirality, is shown. Hydrogen atoms, MeCN solvent molecules and PF_6^- and OTf^- counterions are omitted for the sake of clarity.

5) [3]Catenane 6•8PF$_6$

5.1) Methods

Single crystals of **6**•8PF_6 were grown by slow vapor diffusion of *i*Pr_2O into a solution of the [3]catenane in MeCN at 25 ºC. The single crystals were bathed in inert oil and transferred to the cold gas stream of a Bruker APEX-II CCD diffractometer (CuKα radiation).

5.2) Crystal data

$C_{114}H_{140}F_{48}N_{12}O_{20}P_8Pt_2S_8 \bullet 2CH_3CN$, M = 3886.90, monoclinic, space group $P2_1/n$ (no. 14), a = 35.6937(10), b = 12.3490(4), c = 39.6287(11) Å, β = 99.3191(19)°, V = 17237.1(9) Å^3, T =100.05 K, Z = 4, μ(CuKα) = 5.586 mm^{-1}. A total of 46063 reflections were collected, of which 13568 were unique. Final $wR(F_2)$ = 0.3193. CCDC number: 965478.

There was disordered flurines on P5 restrained with similar distances. Disordered PF_6 anions were constrained to add to 2 whole anions and were refined with group anisotropic displacement parameters.

5.3) Solid-state structure

In the solid-state structure of the [3]catenane **6**•8PF_6 (Figure S22) the organoplatinum square cavity is occupied by the two TTF units both of which adopt the *trans* configuration and are distorted from planarity. The distance between the encapsulated TTF units within the cavity is close to 3.69 Å, while the interplanar separation between the encapsulated TTF units and the plane of the bipyridinium ($BIPY^+$) ranges from 3.45 and 3.62 Å.

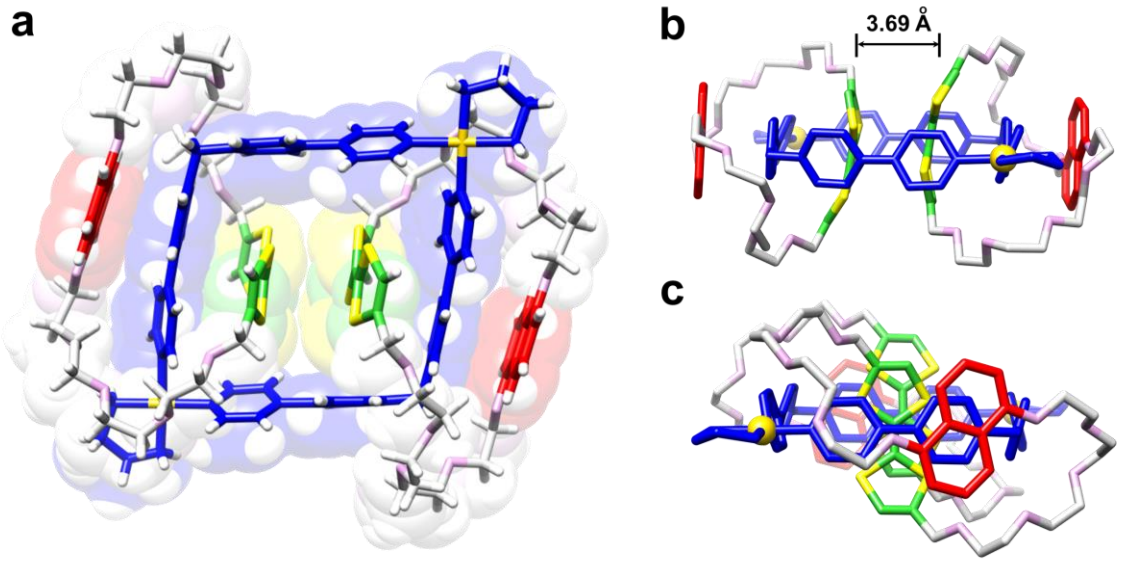


Figure S22. Solid-state structure of the [3]catenane $\mathbf{6}^{8+}$ as (**a)** plan-view in a combined space-filling and stick representation and (**b,c**) two different side-on views in stick representation, along with the average TTF interplanar spacing. Hydrogen atoms, MeCN solvent molecules and PF_6^- counterions are omitted for the sake of clarity.

The DNP units take part in alongside short interplanar contacts with the outer faces of the $BIPY^+$ walls with an average distance of 3.28 Å, which contribute to stabilize the structure together with [C–H···O] hydrogen bonds between some of the glycol oxygens and the $BIPY^+$ hydrogens.

6) Oxidized [3]catenane 6•7PF_6•2ClO_4

6.1) Methods

The oxidised [3]catenane **6**•7PF_6•2ClO_4 was prepared by titration of 1.0 equiv of a solution of $Fe(ClO_4)_3$ in MeCN into a solution of **6**•8PF_6 in MeCN. The formation of mixed-valence state $\mathbf{6}^{9+}$ in solution upon the addition of 1.0 equiv of $Fe(ClO_4)_3$ was monitored by UV-Vis-NIR spectroscopy.

Slow vapor diffusion of Et_2O into the MeCN solution containing $\mathbf{6}^{9+}$ at 0 ºC during two weeks resulted in the separation of red plates of $\mathbf{6}\bullet 7PF_6\bullet 2ClO_4$. The crystals were mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa APEX CCD area detector, equipped with a CuKα microsource with MX optics.

6.2) Crystal data

$C_{130}H_{164}Cl_2F_{42}N_{20}O_{28}P_7Pt_2S_8$, M = 4180.37, triclinic, space group $P\bar{1}$ (no. 2), a = 13.8756(5), b = 17.1561(7), c = 21.5948(8) Å, α = 72.636(2), β = 71.569(2), γ = 68.9620(10)°, V = 4451.5(3) Å^3, T = 99.96 K, Z = 1, μ(CuKα) = 5.579 mm^{-1}. A total of 40651 reflections were collected, of which 13545 were unique (R_{int} = 0.0423). Final $wR(F_2)$ = 0.1857. CCDC number: 965480.

The enhanced rigid-bond restraint (SHELX keyword RIGU) was applied globally. Distance restraints were refined for the disordered PF_6^- counterions.

The solvent masking procedure, as implemented in Olex2, was used to remove the electronic contribution of solvent molecules from the refinement. The formula reports only the atoms used in the refinement. Total solvent accessible volume/cell = 307.2 Å^3 [6.9%] and the total electron count/cell = 24.0.

6.3) Solid-state structure

The stability of the mixed-valence $(TTF)_2^{\bullet+}$ state within the mechanically interlocked framework of the [3]catenane $\mathbf{6}^{9+}$ makes it possible to study the solid-state structure (Figure S23). The structure is surrounded by seven PF_6^- and two ClO_4^- counterions to balance the charge on $\mathbf{6}^{9+}$ in which one of the two tetrathiafulvalene units is in the radical-cationic state.

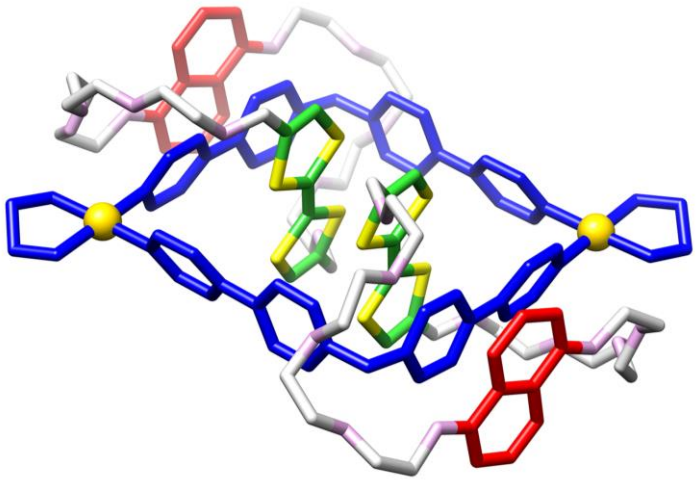


Figure S23. Solid-state structure of the [3]catenane $\mathbf{6}^{9+}$ in the mixed-valence state display as perspective view in stick representation. Hydrogen atoms, MeCN solvent molecules and PF_6^- counterions are omitted for the sake of clarity.

Of particular interest are the relative geometries of the TTF units when comparing the solid-state structure of $\mathbf{6}^{8+}$ and $\mathbf{6}^{9+}$, shown in Figure S24 as two different side-on views which highlights the arrangement of the TTF units in the different oxidation conditions.

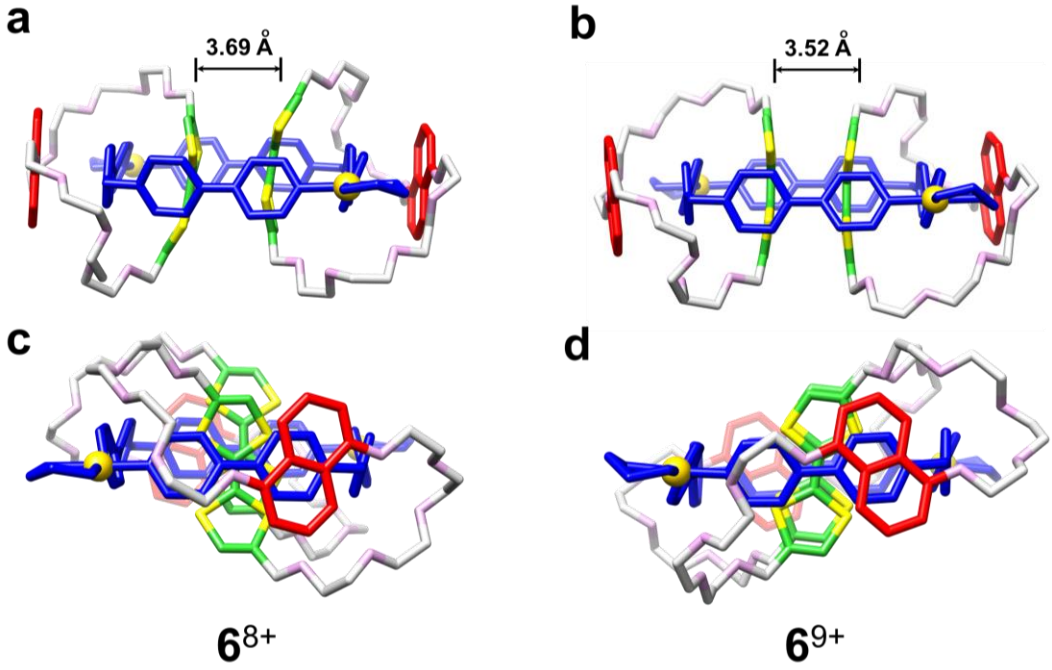


Figure S24. Solid-state structures of (**a,c)** the [3]catenane $\mathbf{6}^{8+}$ and (**b**,**d**) its mixed-valence state $\mathbf{6}^{9+}$ displayed as two different side-on in stick representation. The oxidation of the TTF moieties to the mixed-valence state results in an alteration of the relative arrangement of the TTF units within the organoplatinum square. Hydrogen atoms, MeCN solvent molecules and PF_6^- counterions are omitted for the sake of clarity.

The crystal structure of the ground state of $\mathbf{6}^{8+}$ has (Figure S24a) the TTF units in a slipped-stack arrangement with a vertical offset, measured as offset between the planes of the TTF units, of 1.6 Å and a negligible angular offset, define as relative orientation of the C=C double bounds in the TTF units, of 0.2° between the two TTF units. This arrangement change (Figure S24b) in the mixed-valence $(TTF)_2^{\bullet+}$ state where the TTF units overlaps almost perfectly with no angular and vertical offset.

7) [3]Catenane 9•8PF$_6$

4.1) Methods

Single crystals of $\mathbf{9}\cdot 8PF_6$ were grown by slow vapor diffusion of iPr$_2$O into a solution of the [3]catenane in MeCN at 25 ºC. The single crystals were bathed in inert oil and transfered to the cold gas stream of a Bruker APEX-II CCD diffractometer (CuKα radiation).

4.2) Crystal data

$C_{114}H_{140}F_{48}N_{12}O_{20}P_8Pd_2S_8$, M = 3627.41, monoclinic, space group C2/c (no. 15), a = 35.8988(19), b = 12.3423(6), c = 39.878(2) Å, β = 100.002(4)°, V = 17400.5(16) Å^3, T =99.99 K, Z = 4, μ(CuKα) = 4.221 mm^{-1}. A total of 24963 reflections were collected, of which 8228 were unique. Final $wR(F_2)$ = 0.3771. CCDC number: 965480.

Distance restraints were refined for the disordered PF^-_6 counterions. The solvent masking procedure, as implemented in Olex2, was used to remove the electronic contribution of solvent molecules from the refinement. The formula reports only the atoms used in the refinement. Total solvent accessible volume/cell = 2735.0 Å^3 [15.7%] Total electron count/cell = 616.5.

4.3) Solid-state structure

In the X-ray crystal structure of the [3]catenane $\mathbf{9}^{8+}$ (Figure S21) both TTF units are housed within the cavity of the organopalladium square cavity and stabilized by a combination of [π···π] donor-acceptor and [C–H···O] interactions.

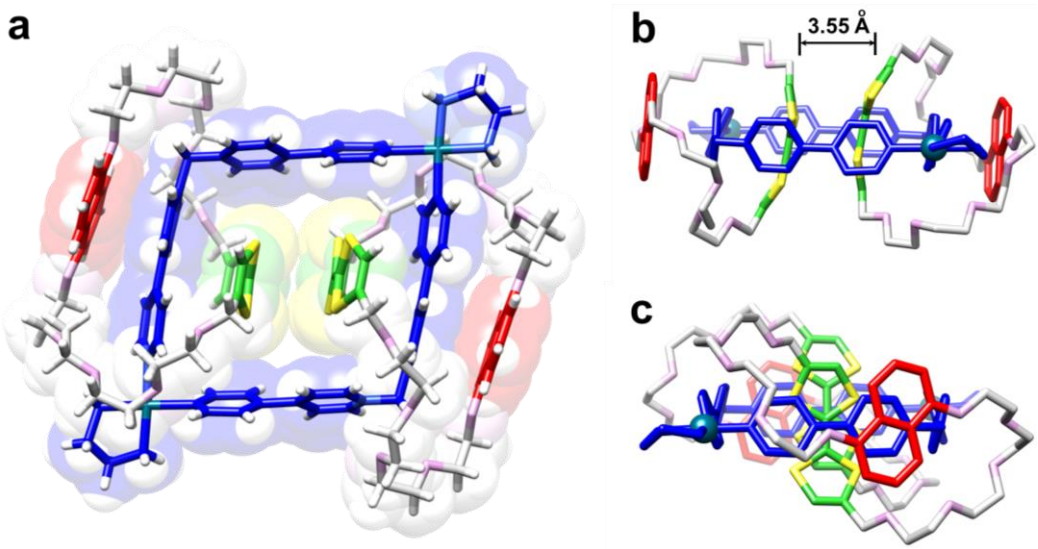


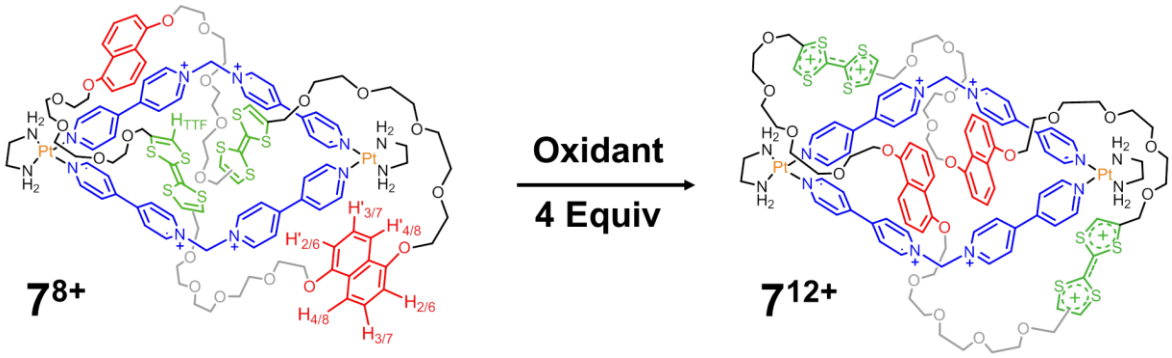
Figure S25. Solid-state structure of the [3]catenane $\mathbf{9}^{8+}$ assembled from the ligand $\mathbf{2}\cdot 2PF_6$ with ethylenediamine Pt(II) metal center **5** in the presence of two electron-rich aromatic crown ether **3**, as (**a)** plan-view in a combined space-filling and stick representation and (**b,c**) two different side-on views in stick representation, along with the average TTF interplanar spacing and the angle of offset, defined by the relative orientations of the C-C double bonds in the TTF units. Hydrogen atoms, MeCN solvent molecules and PF_6^- counterions are omitted for the sake of clarity.

The values of the interplanar distance (3.55 Å) and the orientation of the tetrathiafulvalene units within the molecular framework of the [3]catenane $\mathbf{9}^{8+}$ are very similar to the ones observed for the [3]catenane $\mathbf{6}^{8+}$ where the two TTF units are contained in the organoplatinum square.

E. Spectroscopic and Electrochemical Switching Studies

1) NMR Spectroscopic analysis

The precise and quantitative nature of the redox-controlled switching process undergone (Scheme S6) by the molecular Solomon link $\mathbf{7}^{8+}$ was probed using ^{1}H NMR spectroscopy. The chemical oxidation of $\mathbf{7}^{8+}$ to $\mathbf{7}^{12+}$ was performed in CD_3CN using tris-4-bromophenylimminium hexachloroantimonate as the chemical oxidant. After recording the spectrum of a solution of **7**•8PF_6 in CD_3CN at 233 K, 4.5 equiv of oxidant was added to the sample and the temperature was lowered quickly to 233 K and the spectrum was recorded once again. Examination of the spectrum of the oxidized sample provides evidence for the complete oxidation of both TTF units to their dicationic TTF^{2+} form. Two peaks corresponding to TTF^{2+} can be identified at 9.2 and 9.4 ppm.



Scheme S6. Structural formulae of the molecular Solomon link $\mathbf{7}^{8+}$ and its oxidised form $\mathbf{7}^{12+}$.

Evidence for the sliding of the macrocyclic polyether switching from the TTF to the DNP recognition sites being located within the organoplatinum square upon oxidation is apparent from the observation of the upfield shifts of the peaks corresponding to the protons of the DNP unit. The ^{1}H NMR spectrum, along with the ^{1}H–^{1}H COSY (Figure S26) and ^{1}H–^{1}H ROESY spectrum (Figure S27) of the oxidized $\mathbf{7}^{12+}$, shows clearly the scalar coupling between the protons on the DNP units. Moreover, the ^{1}H NMR spectrum of oxidised $\mathbf{7}^{12+}$ does not show signals corresponding to the "uncomplexed" DNP unit or TTF^{2+} ions housed in the organoplatinum square. This result confirms that, within the detection limit of the ^{1}H NMR spectroscopy, the switching of the molecular Solomon link between its ground and fully oxidized state is quantitative. Analysis by diffusion-ordered NMR spectroscopy (DOSY) confirmed (Figure S29) the presence of a single species; the diffusion coefficient *D* (1.6×10^{-10} $m^2 \cdot s^{-1}$) for the oxidized $\mathbf{7}^{12+}$ is very close to the *D* coefficient (1.8×10^{-10} $m^2 \cdot s^{-1}$) measured for the reduced $\mathbf{7}^{8+}$.

1.1) ^{1}H– ^{1}H COSY Spectrum

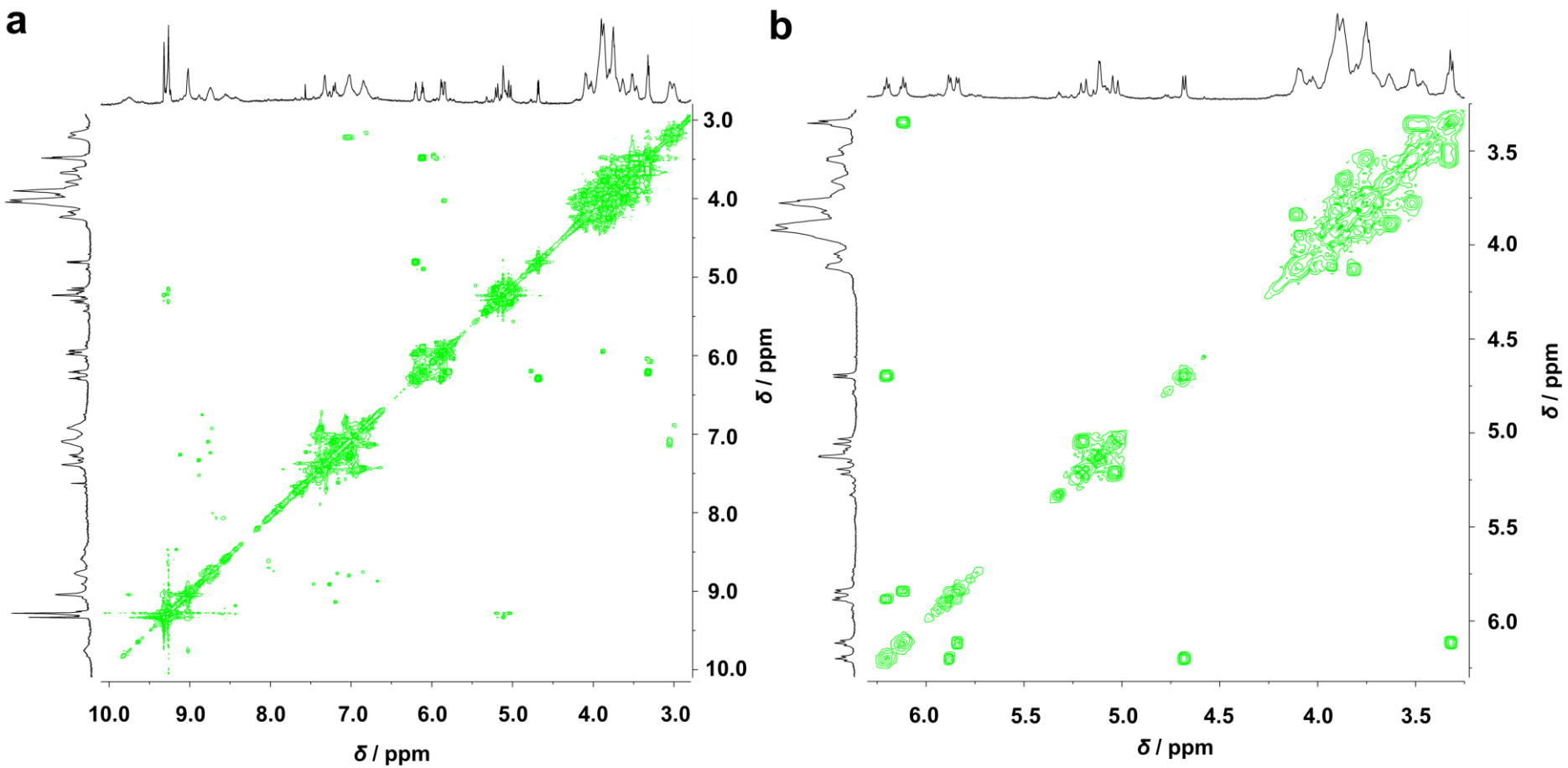


Figure S26. ^{1}H–^{1}H COSY Spectrum (600 MHz, CD_3CN, 233 K) of **7**•$8PF_6$•$4ClO_4$ (**a**) in the full region and (**b**) expanded to 3.5–6.5 ppm.

1.2) $^{1}H–^{1}H$ ROESY Spectrum

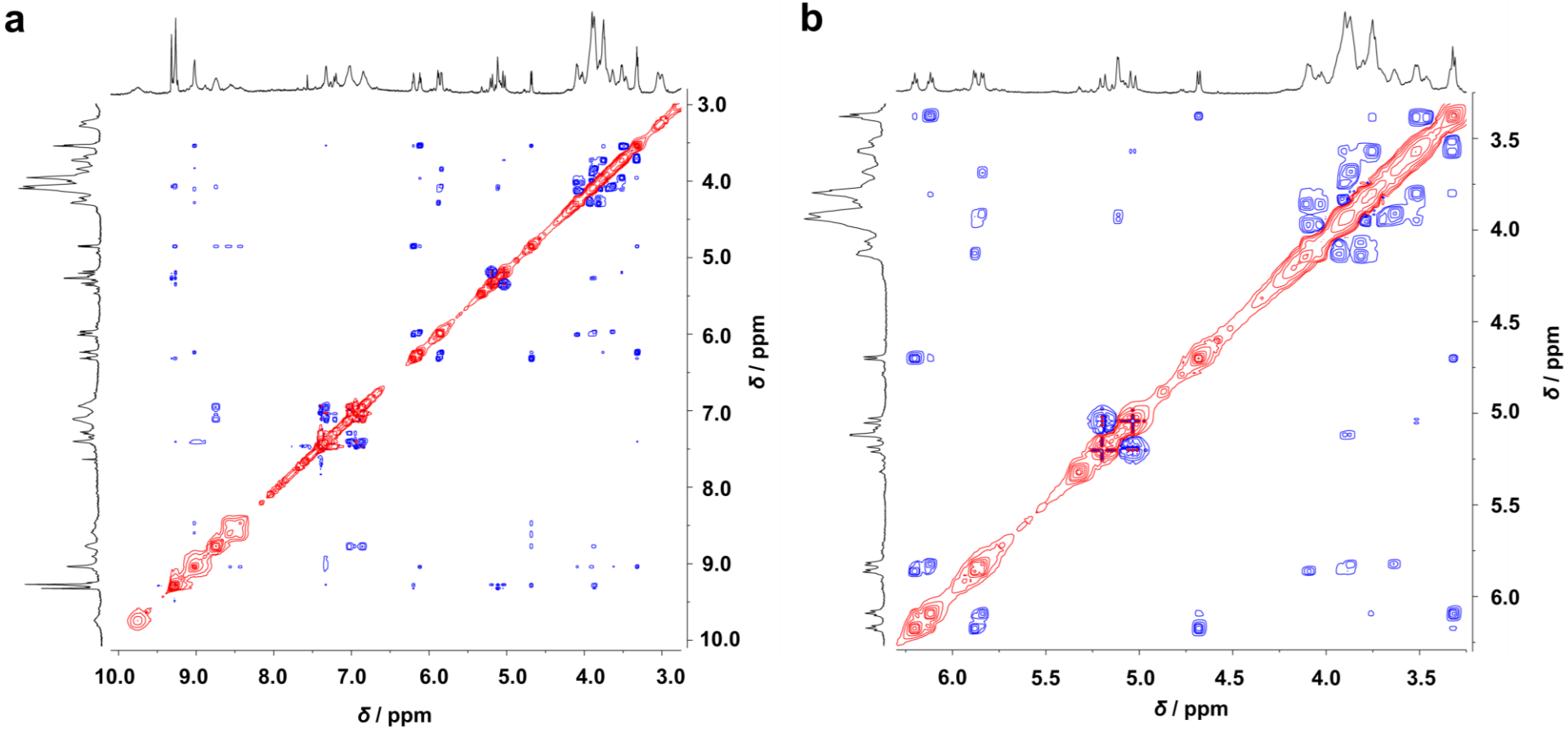


Figure S27. $^{1}H–^{1}H$ ROESY Spectrum (600 MHz, CD_3CN, 233 K) of **7**•8PF_6•4ClO_4 (**a**) in the full region and (**b**) expanded to 3.5–6.5 ppm.

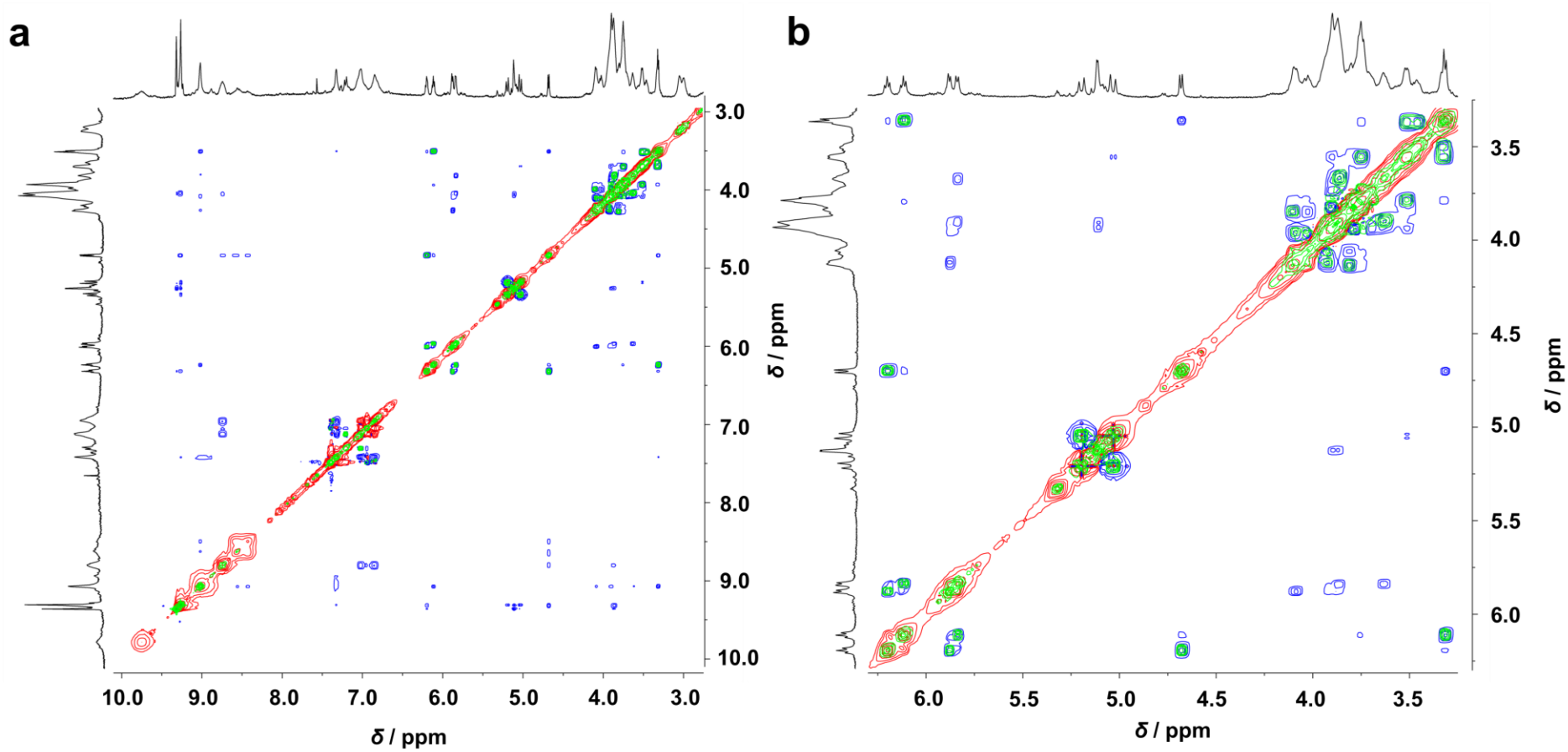


Figure S28. ^{1}H–^{1}H COSY overlap with ^{1}H–^{1}H ROESY spectrum (600 MHz, CD_3CN, 233 K) of **7**•8PF_6•4ClO_4 (**a**) full and (**b**) expanded to 3.5–6.5 ppm.

1.3) ^{1}H DOSY NMR Spectrum

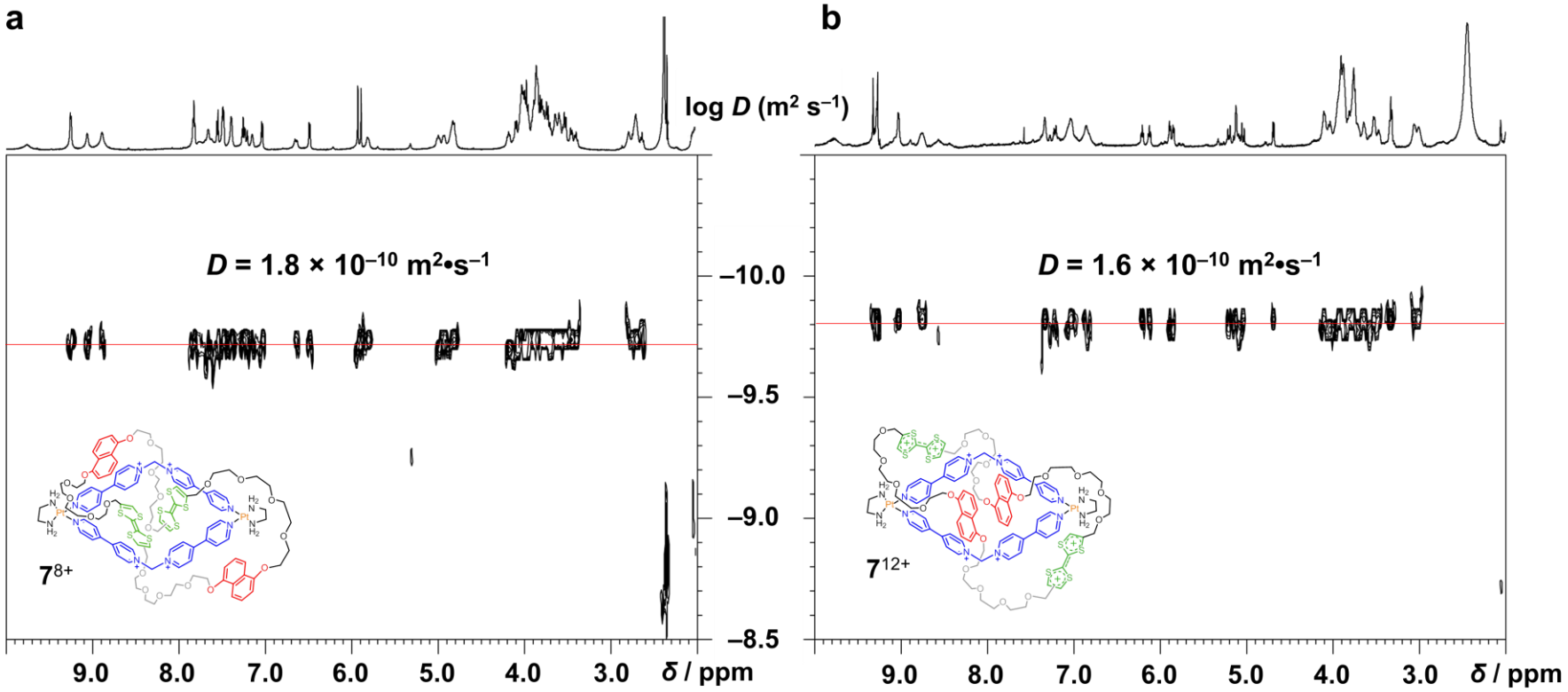


Figure S29. ^{1}H DOSY NMR spectrum (600 MHz, CD_3CN, 233 K) of (**a**) **7**•8PF_6 and (**b**) **7**•8PF_6•4ClO_4 recorded following the addition of 4 equiv of tris(4-bromophenyl)ammoniumyl hexachloroantimonate.

2) Electrochemical studies

2.1) Cyclic voltammetry

The redox-controlled switching of $\mathbf{7}^{8+}$ was investigated (Figure S30) by cyclic voltammetry (CV) in MeCN with $TBAPF_6$ as the electrolyte. The oxidation of the TTF units in $\mathbf{7}^{8+}$ resulted (Figure S31) in two peaks at +581 mV (I) and +830 mV (II) versus Ag/AgCl. The first oxidation peak can be assigned to the formation of a stable species, such as the TTF mixed-valence dimer $(TTF)_2^{\bullet+}$. The second broad anodic peak reveals, not only a stepwise mechanism for the oxidation of the tetrathiafulvalene units from the mixed-valence state to the TTF^{2+} dicationic form, but also the presence of an equilibrium between the tetrathiafulvalene units in the radical-cation form and the DNP units being located within the molecular Solomon link.

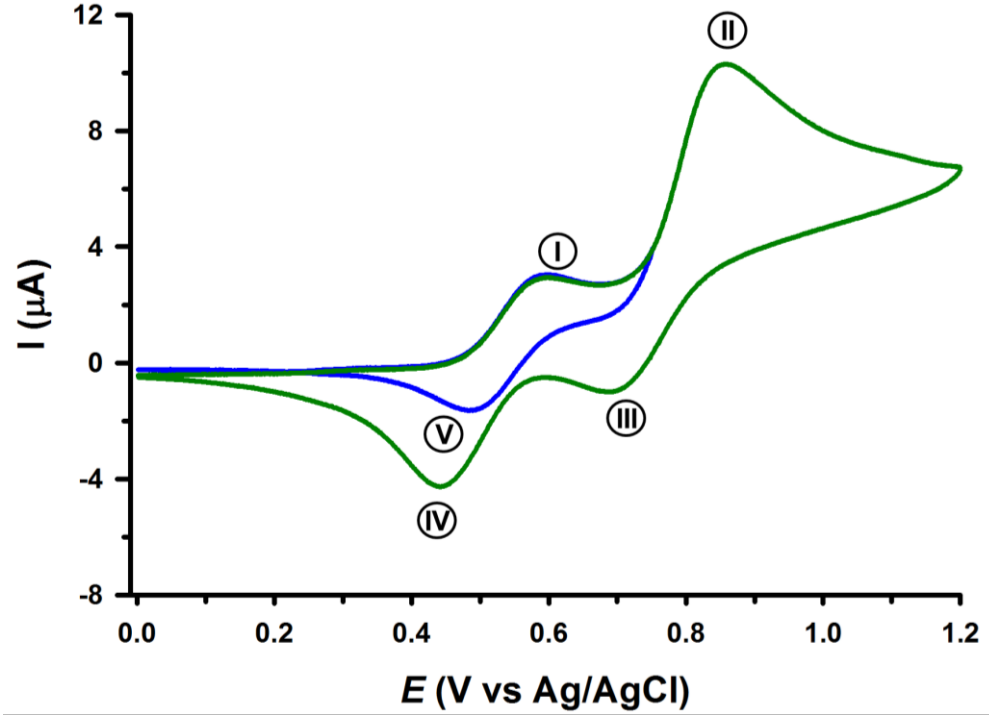


Figure S30. Cyclic voltammograms (1 mM in MeCN, 100 mM $TBAPF_6$, 10 $mV \cdot s^{-1}$, 298 K) of the molecular Solomon link **7**•$8PF_6$ recorded at two different vertex potentials.

The characteristic reduction peaks observed during the cathodic sweep, indicate the reduction of the dicationic TTF^{2+} units to the radical-cation and subsequently back to the neutral form. When the scan direction of the voltammogram is switched back at a vertex potential of +750 mV, a one-electron reduction process is observed. This redox process is independent of the scan rate and is totally reversible (Figure S31a). These results suggest that a stable specie is

formed upon the ejection of one electron from the TTF unit that can be ascribed to the generation of the TTF mixed-valence dimer $(TTF)_2^{\bullet+}$.

The second oxidation peak displays (Figure S31b) scan-rate-dependent behavior. At a low scan rate, a broad three-electron oxidation peak is observed. At a faster scan rate, it becomes clear that the oxidation occurs by two different processes.

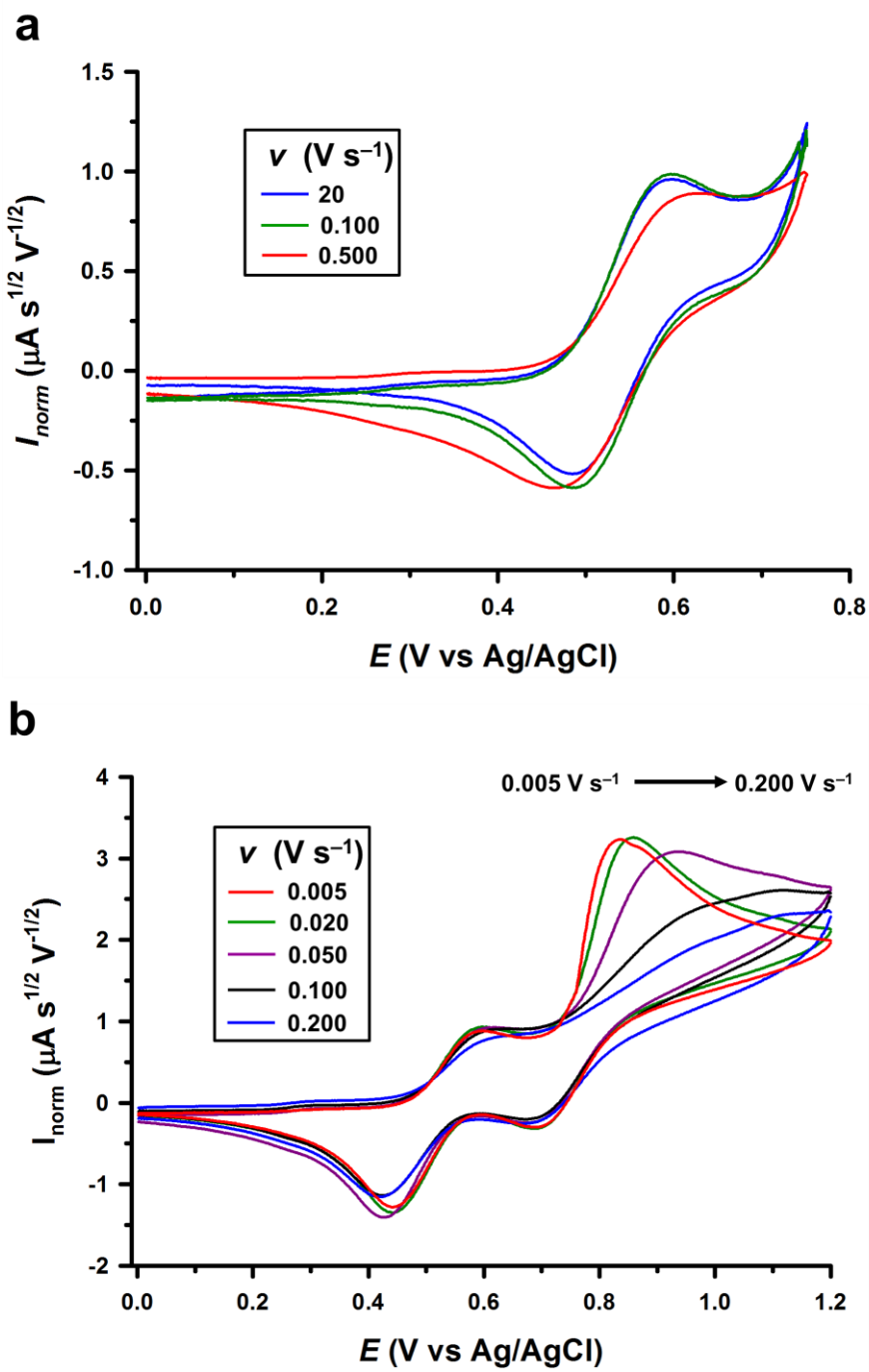


Figure S31. Variable scan-rate cyclic voltammograms (1 mM in MeCN, 100 mM $TBAPF_6$, 298 K) of the molecular Solomon link **7**•$8PF_6$ recorded in the range of (**a**) 0 to 750 mV, and (**b**) 0 to 1100 mV.

The shift of the oxidation potential towards more positive values at increasing scan rate points to the existence of an equilibrium between the $\mathbf{7}_{in}^{10+}$ state, where both $TTF^{\bullet+}$ units are housed within the cavity of the organoplatinum square and the co-conformation $\mathbf{7}_{out}^{10+}$ in which both of them leave the cavity on account of the destabilizing electrostatic interactions. Attempts to measure the oxidation of both $TTF^{\bullet+}$ units to TTF^{2+} inside the cavity at higher scan rates were hindered by the irreversible oxidation of the DNP groups at higher potentials. We have carried out cyclic voltammetry experiments in MeCN of the [3]catenane **6**•8PF_6 in order to investigate the switching mechanism of this molecule (Figure S32). Examination of the cyclic voltammogram reveals one-electron oxidation occurring at +593 mV which is assigned to the mixed-valence state. The second oxidation event, at +750 mV, corresponds to the formation of two radical-cation $TTF^{\bullet+}$ units and it is 70 mV easier to oxidase compared to the same redox process observed in the molecular Solomon link **7**•8PF_6.

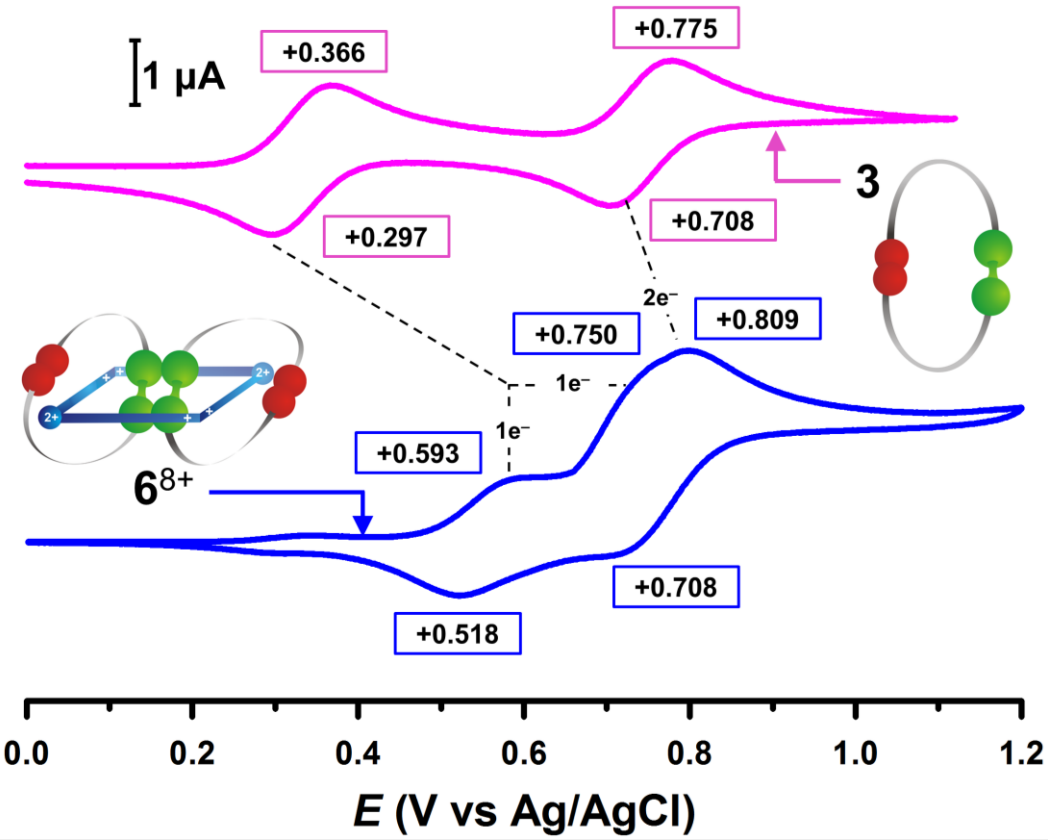


Figure S32. Cyclic voltammograms (1 mM in MeCN, 100 mM $TBAPF_6$, 10 $mV \cdot s^{-1}$, 298 K) of the TTF-DNP macrocycle **3** (pink curve) and the [3]catenane **6**•8PF_6 (blue curve). The voltammogram of $\mathbf{6}^{8+}$ shows three oxidation peaks, two one-electron and one two-electrons processes, occurring with peak potential at 0.593, 0.750 and 0.809 V versus Ag/AgCl.

The final oxidation potential of $\mathbf{7}^{10+}$ at +809 mV, where the oxidation from $TTF^{\bullet+}$ to TTF^{2+} occurs, does not exhibit a significant shift when compared to the second oxidation potential of the TTF-DNP macrocycle **3**. This result indicates the formation of an equilibrium between the radical-cation dimer $(TTF^{\bullet+})_2$ inside the organoplatinum square, $\mathbf{6}_{in}^{10+}$, and the $\mathbf{6}_{out}^{10+}$ state where both $TTF^{\bullet+}$ leave the cavity by circumrotation of the macrocycle. Variable scan rate voltammograms provide (Figure S33) further evidences for the existence of this equilibrium.

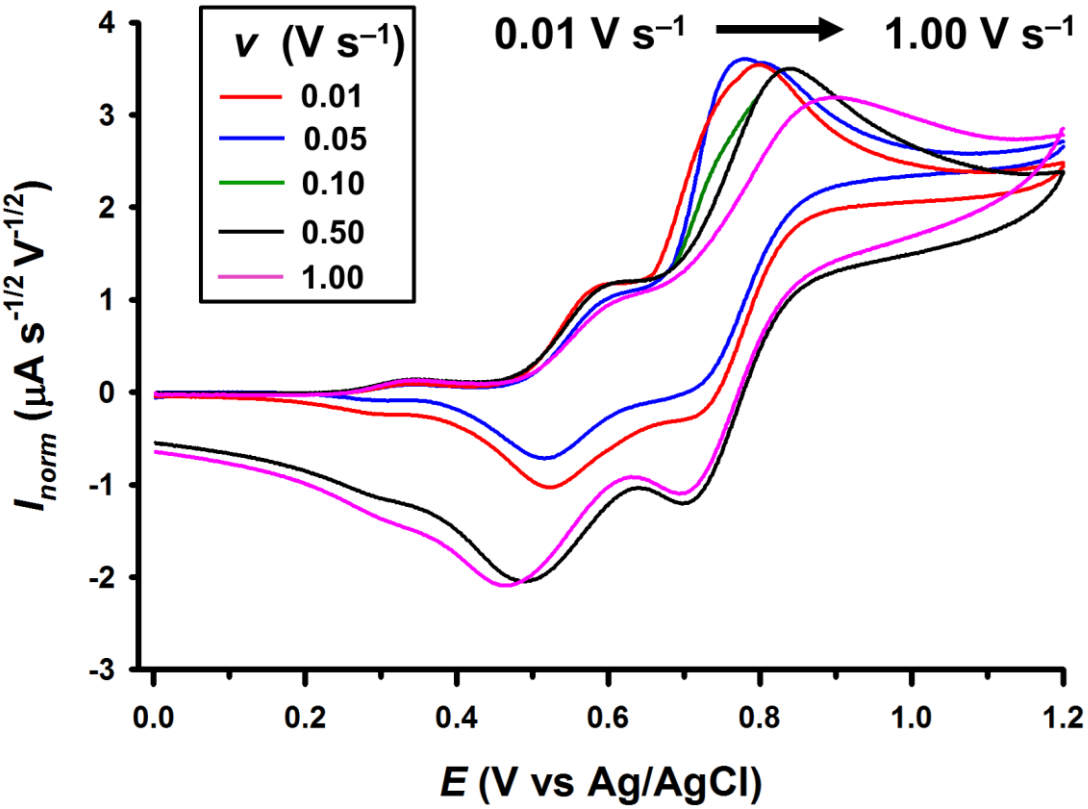


Figure S33. Variable scan-rate cyclic voltammograms (1 mM in MeCN, 100 mM $TBAPF_6$, 298 K) of the [3]catenane **6**•$8PF_6$ recorded in the range 10 to 1100 mV.

In the slow scan regime, if enough time is given to the $TTF^{\bullet+}$ units to leave the organoplatinum square by circumrotation of the two crown ethers and an equilibrium is established between the $\mathbf{6}_{in}^{10+}$ and $\mathbf{6}_{out}^{10+}$ state, the oxidation of TTF occurs outside the organoplatinum square at +809 mV. In the fast scan regime (>1 V s^{-1}), the intensity of the peak at +809 mV decrease and the peak is shifted toward more positive potentials, which indicate that there is not enough time for the equilibration to occurs.

2.2) Chronocoulometry

Chronocoulometry experiments were performed (Figure S34) on a MeCN solution of the molecular Solomon link **7**•8PF_6 in order to determine quantitatively the number of electrons involved in each redox process. The analysis of the chronocoulometric data was performed with the Anson equation,[S6] which defines the charge-time dependence for linear diffusion control processes:

$$Q = 2nFACD^{1/2}\pi^{1/2}t^{1/2}$$

where Q is the amount of charge, n is the number of electrons transferred per molecule, F is the Faraday's constant (96500 C mol^{-1}), A is the electrode area (cm^2), C is the concentration (mol cm^{-3}) and D is the diffusion coefficient (cm^2 s^{-1}). Since all these parameters are known and a linear relationship exists between Q and $t^{1/2}$, the number of electrons can be calculated from the slope of the Anson plot.

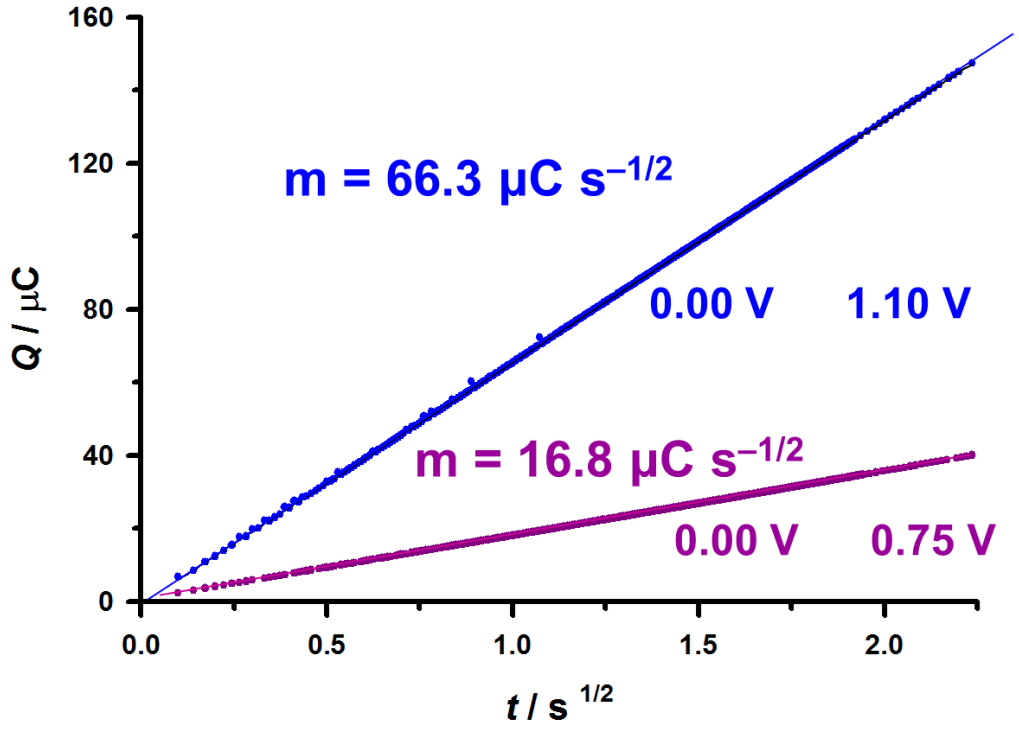


Figure S34. Anson plot of the chronocoulometry experiments (1 mM in MeCN, 100 mM $TBAPF_6$, 298 K) performed on the molecular Solomon link **7**•8PF_6. The potential was set from 0 to 750 mV (purple line), and from 0 to 1100 mV (blue line).

The charge resulting from the first process was measured by setting the potential from 0 to +750 mV, giving a slope from the Anson plot of 16.8 µC $s^{-1/2}$.

The potential was then set from 0 to +1100 mV and a slope of 66.3 μC $s^{-1/2}$ was obtained from the charge transferred for both redox processes. The ratio of the slopes of the best-fit lines for the second process with respect to the first one was found equal to 4.1. If we consider the number of electrons transferred per molecule, the first redox process is a one-electron process which furnishes the mixed-valence dimer $(TTF)_2^{\bullet+}$ state, while the second one is a three-electron process.

3) Spectroelectrochemistry experiments

The switching mechanism of the molecular Solomon link was examined by UV-Vis-NIR adsorption spectroscopy of the electrochemically generated species. The spectroscopic changes associated with the oxidation of a 0.15 mM solution of **7**•8PF_6 in MeCN (with 100 mM $TBAPF_6$) were recorded (Figure S35) over a range of potentials.

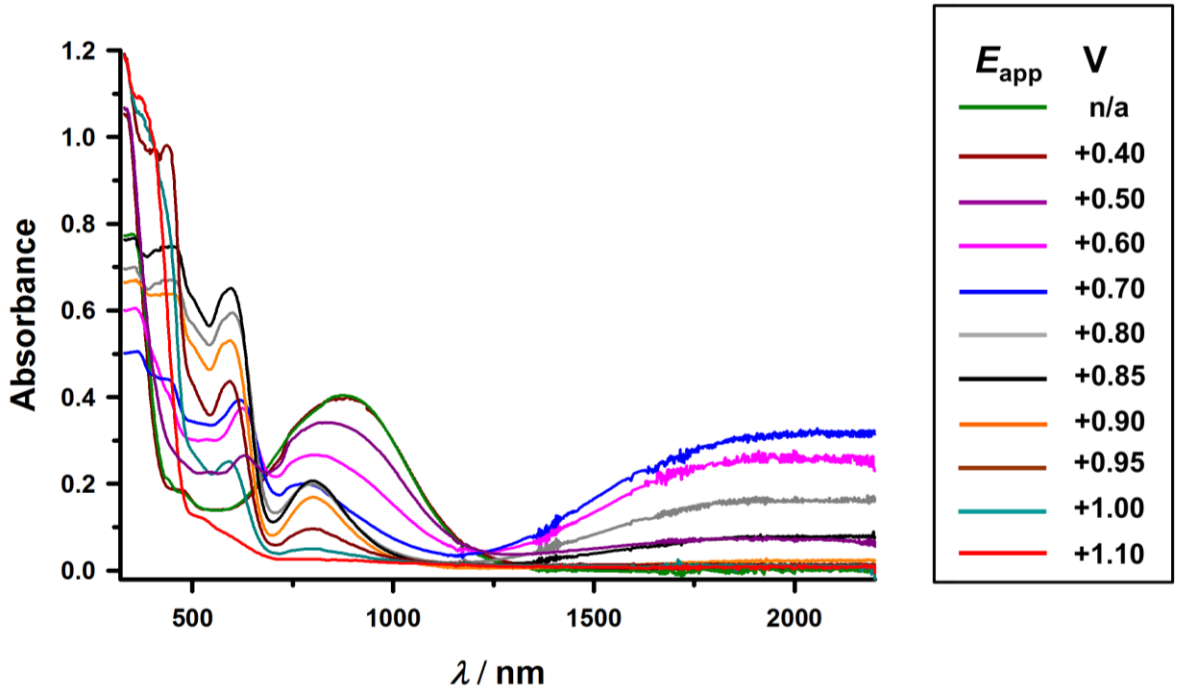


Figure S35. UV-Vis-NIR spectroelectrochemistry of **7**•8PF_6 (0.15 mM in MeCN, 100 mM $TBAPF_6$, 298 K) recorded over a range of potentials (versus Ag/AgCl).

Application of oxidation potentials from +400 to +700 mV versus Ag/AgCl resulted in the gradual decrease of the charge-transfer adsorption band at 860 nm. This band is replaced by the characteristic bands for the radical-cation $TTF^{\bullet+}$ at 620 nm and 437 nm. These changes were accompanied by the appearance of a broad NIR band around 2000 nm, which is a signature for the formation of the mixed-valence $(TTF)_2^{\bullet+}$ state in $\mathbf{7}^{9+}$.

Upon oxidation over more positive potentials, the intervalence band at 2000 nm slowly blanches, while the $TTF^{\bullet+}$ adsorption bands continue to increase until they reach a maximum intensity at an applying potential of +850 mV. The increases in intensity of these two bands is associated with the oxidation of both TTF units to their radical-cationic form. The presence of an adsorption band at 800 nm can be attributed to the formation of radical-cation $(TTF^{\bullet+})_2$ dimer within the organoplatinum square. The absorption band measured in this case is weaker compared with that of the previously reported[S7] radical-cation dimer of tetrathiafulvalene, an observation which suggests the presence of an equilibrium between the $\mathbf{7}_{in}^{10+}$ state, where both $TTF^{\bullet+}$ units are enclosed inside the structural framework of the organoplatinum square as the radical-cation dimer, and the $\mathbf{7}_{out}^{10+}$ state in which both of them have left the cavity on account of the destabilizing electrostatic interactions. Application of more positive potentials results in the gradual decrease in intensity of the radical-cation $TTF^{\bullet+}$ adsorption peaks and the appearance of the characteristic TTF^{2+} dication adsorption band at 370 nm. The complete oxidation of the tetrathiafulvalene to their dicationic states reveals a new adsorption band around 600 nm, which can be assigned to the charge-transfer of the organoplatinum square encircling the DNP units.

The spectroscopic changes with time of electrolysis were also recorded (Figure S36a-c). The changes in the adsorption spectra at different applied potentials support the generation of different oxidation states of the molecular Solomon link. Furthermore, the switching ability of molecule between the reduced $\mathbf{7}^{8+}$ state and the fully oxidized $\mathbf{7}^{12+}$ form was evaluated (Figure S36d). Indeed, the original spectrum of $\mathbf{7}\bullet 8PF_6$ with the characteristic charge-transfer band at 860 nm was restored after rereduction of the fully oxidized $\mathbf{7}^{12+}$ state by holding the potential at 0 V for 1 h, demonstrating the reversibility of the switching process.

Spectroelectrochemistry was performed (Figure S37) on a MeCN solution of the [3]catenane $\mathbf{6}^{8+}$ in order to shed more light on the optical properties associated with the redox processes. Indeed substantial changes occur in the UV-Vis-NIR spectrum of $\mathbf{6}^{8+}$ upon electrochemical oxidation. The broad TTF–$BIPY^+$ charge transfer adsorption band at 890 nm decrease on setting the voltage of the electrode at +650 mV versus Ag/AgCl, while a brad NIR signal appear at *ca*. 2000 nm, as expected for the formation of the mixed-valence $(TTF)_2^{\bullet+}$ state. By applying a potential of +760 mV, a band around 800 nm was observed, while the NIR absorption band completely disappeared. The new band can be attributed to the generation of the radical-cation dimer $(TTF^{\bullet+})_2$ state inside the organoplatinum square. The fully oxidation to the $\mathbf{6}^{12+}$ state was achieved by applying a potential of +1100 mV which is associated with the appearance of a band around 400 nm, characteristic of the TTF^{2+} dication.

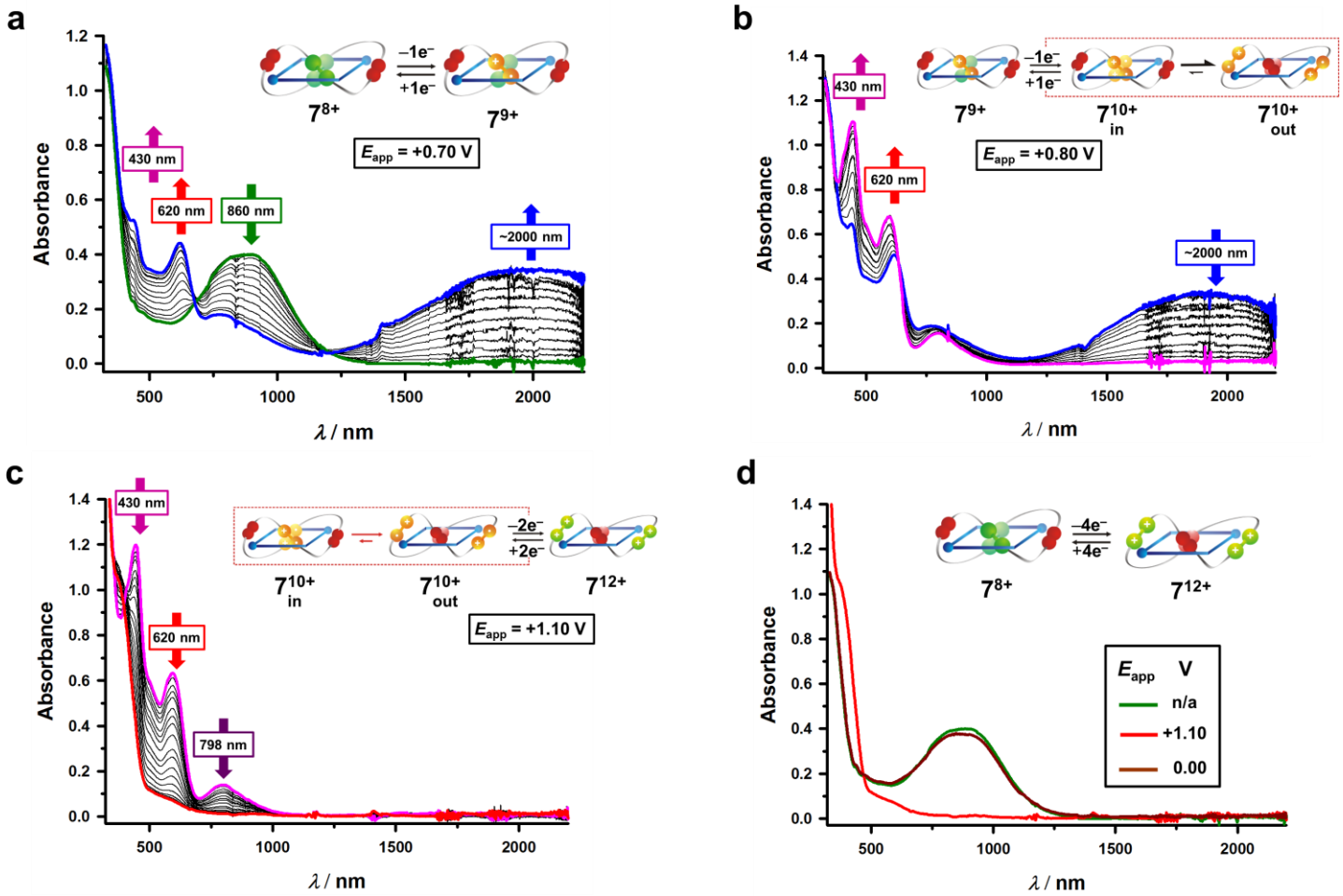


Figure S36. UV-Vis-NIR Spectroelectrochemistry performed on a solution of **7**•8PF_6 (0.15 mM in MeCN, 100 mM $TBAPF_6$, 298 K) recorded at (**a**) +0.70, (**b**) +0.80, and (**c**) +1.10 V versus Ag/AgCl. The spectra at each applied potential were measured every 2 min. (**d**) UV-Vis-NIR Spectra recorded during the exhaustive four-electron oxidation of $\mathbf{7}^{8+}$ at +1.10 V, showing the replacement of the TTF charge-transfer adsorption band at 860 nm by the adsorption arising from the inclusion of the DNP units inside the organoplatinum square. The original adsorption band is regained after exhaustive reduction at 0 V.

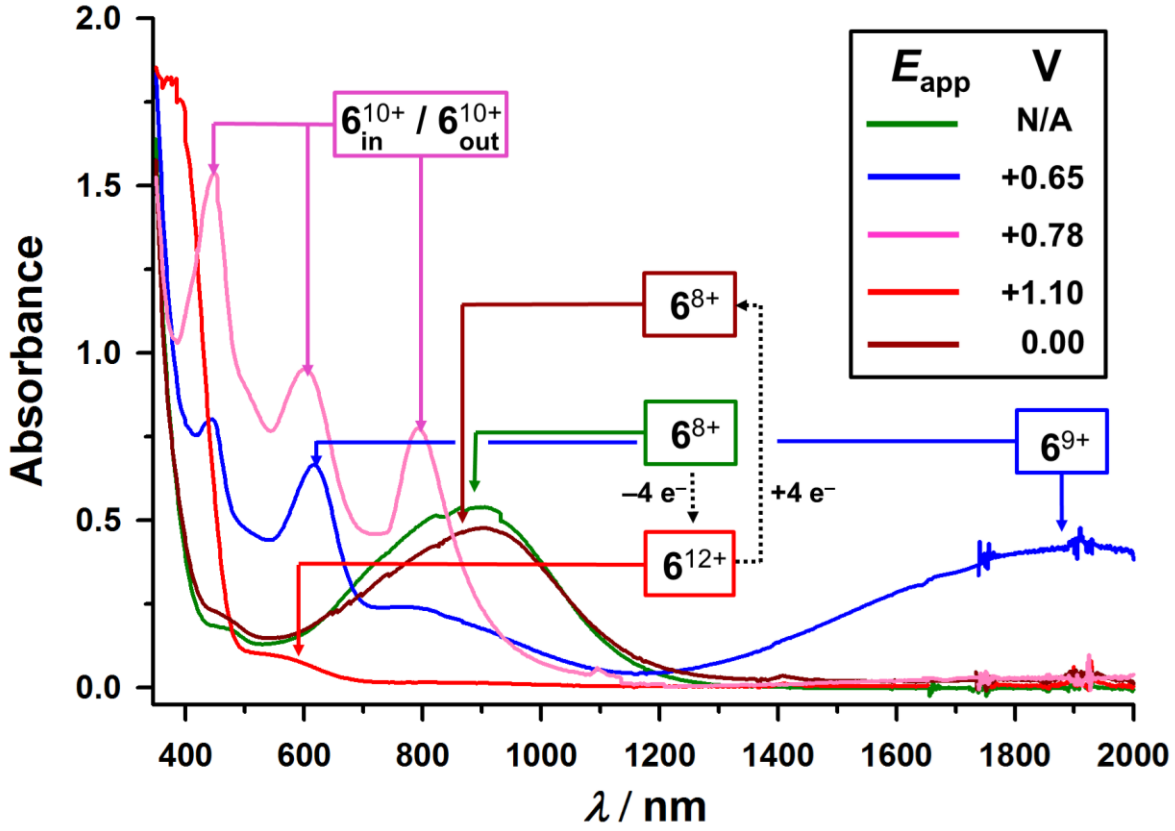


Figure S37. UV-Vis-NIR Spectroelectrochemistry performed on a solution of **6**•8PF_6 (0.15 mM in MeCN, 100 mM $TBAPF_6$, 298 K) recorded at (**a**) +0.65, (**b**) +0.75, and (**c**) +1.10 V versus Ag/AgCl. The original spectrum of $\mathbf{6}^{8+}$ is regained after sustained reduction at 0 V.

The UV-Vis-NIR spectroscopic changes were also investigated (Figure S38) for the macrocyclic polyether **4** at different applied potentials. The electrolysis of a 0.15 mM solution of **4** in MeCN at + 0.70 V results (Figure S38a) in the formation of an intramolecular $TTF^{\bullet+}$ radical-dimer interaction occurring within the macrocyclic polyether,[S1] as indicated by the growth of the visible bands at 540 and 800 nm. In addition to those bands, the characteristic adsorption peaks of the radical-cation $TTF^{\bullet+}$ were observed at 400 and 560 nm. After holding the potential at +1.1 V, the $TTF^{\bullet+}$ radical-dimer bands experienced (Figure S38b) a decrease in intensity. A broad peak center on 800 nm which was assigned[S1] to the intramolecular charge-transfer band between the oxidized TTF^{2+} units and the DNP units appears after complete oxidation of TTF to the dicationic state.

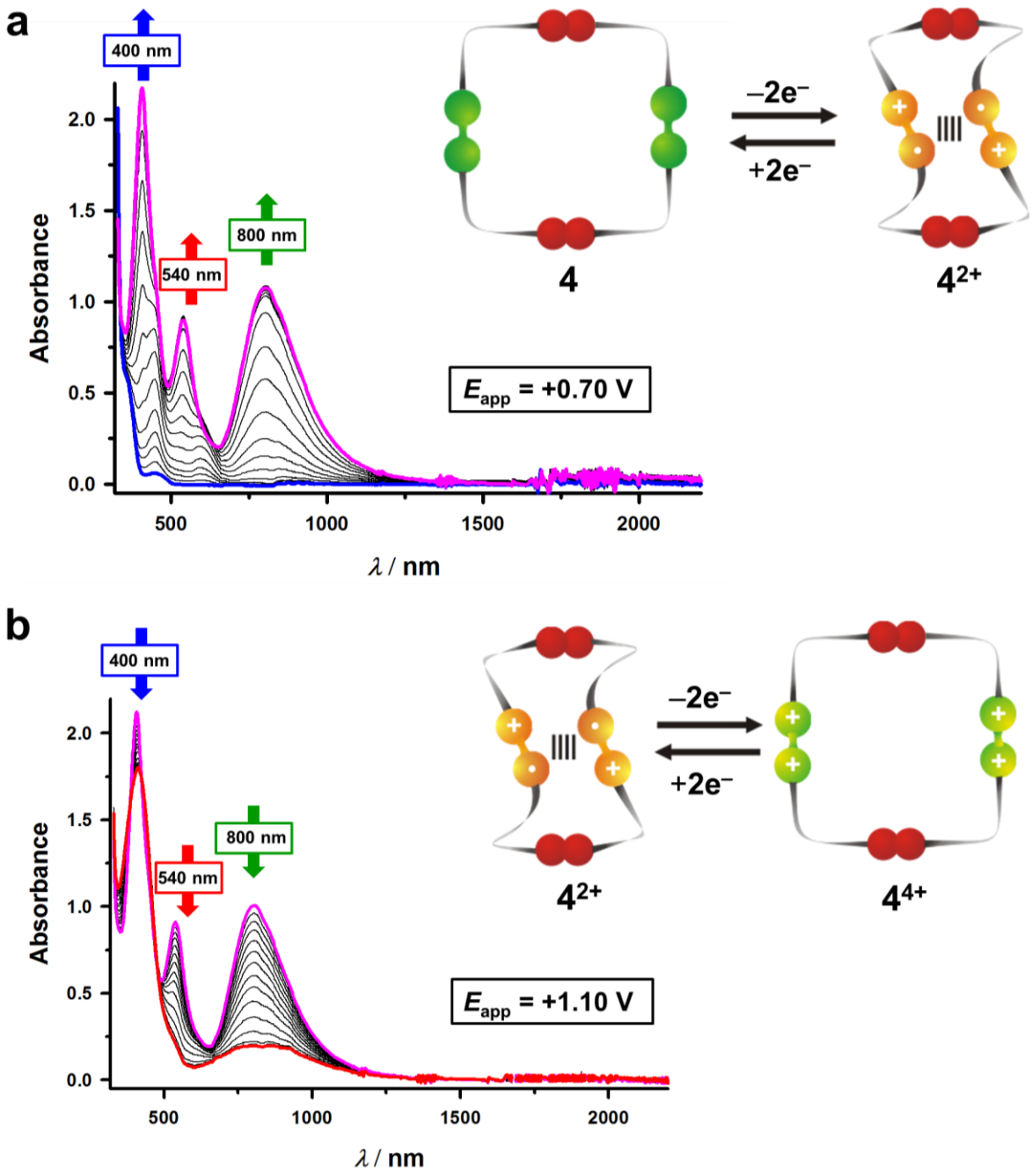


Figure S38. UV-Vis-NIR Spectroelectrochemistry performed on the macrocyclic polyether **4** (0.15 mM in MeCN, 100 mM $TBAPF_6$, 298 K) after electrolysis at (**a**) +0.70 V and, (**b**) +1.10 V versus Ag/AgCl.

Spectroelectrochemical experiments were also carried out on the ring-in-ring complex obtained by mixing the macrocyclic polyether **4** and the preformed organoplatinum square $\mathbf{8}^{8+}$. The adsorption spectrum (Figure S39) of a 0.15 mM solution of the 1:1 complex in MeCN after electrolysis at +0.70 and +1.10 V reveals similar features to those observed in the spectrum of the oxidized macrocyclic polyether.

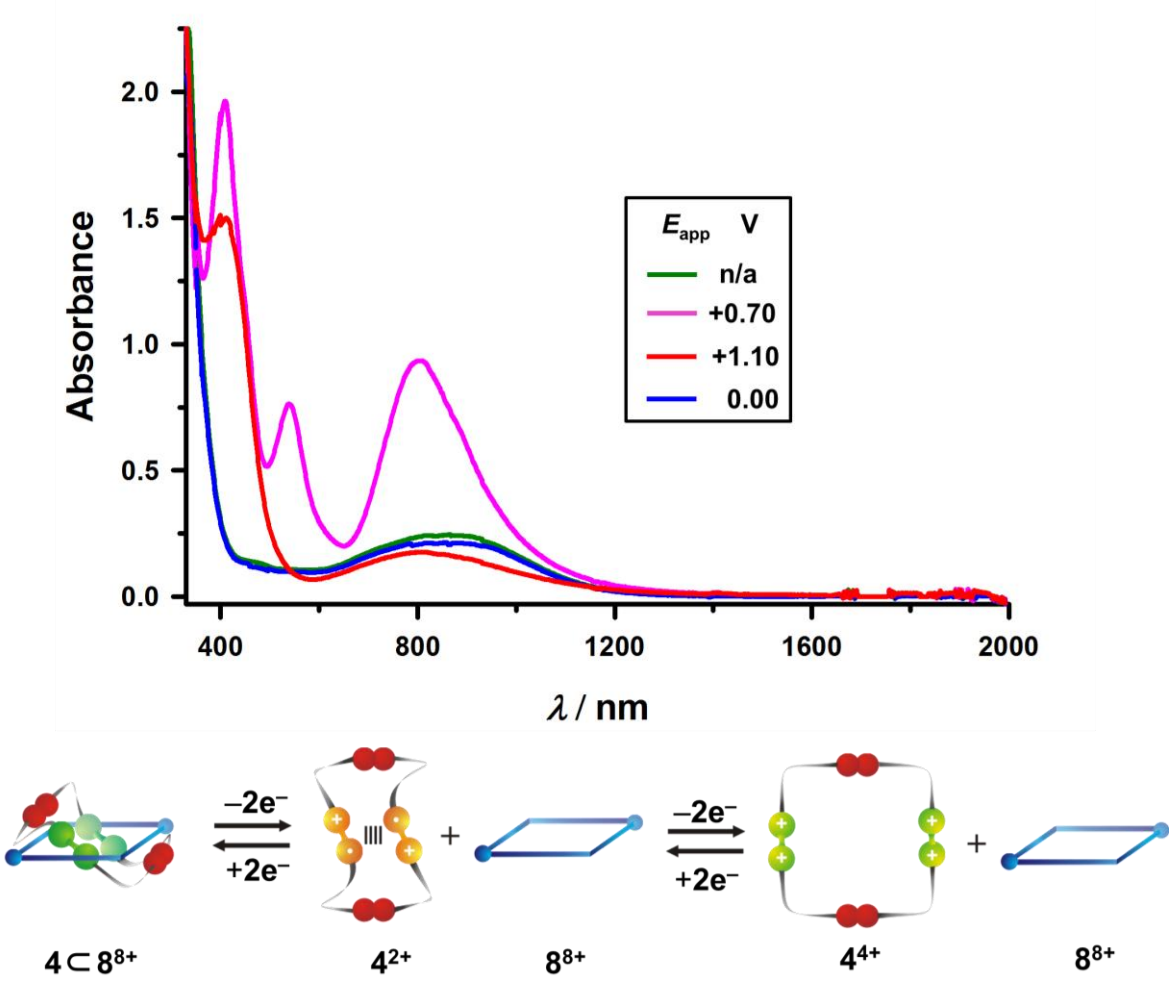


Figure S39. UV-Vis-NIR Spectroelectrochemistry of the 1:1 mixture of **4** and **8**•8PF_6 (0.15 mM in MeCN, 100 mM $TBAPF_6$, 298 K) recorded at different potentials (vs Ag/AgCl).

These results indicate that the ejection of **4** from the organoplatinum square occurs immediately upon oxidation of the TTF units to their radical-cations as a result of severe electrostatic repulsion between the two components. Finally, the original 1:1 complex is restored after re-reduction of the TTF^{2+} dications to their neutral forms, as indicated by the regeneration of the charge-transfer band at 856 nm.

4) Electron Paramagnetic Resonance (EPR) Spectroscopy

EPR Spectroscopy was performed in order to investigate the mechanism of redox switching of the molecular Solomon link. The different redox species were generated by electrochemical oxidation or by titrating the chemical oxidant $Fe(ClO_4)_3$ into a MeCN solution of **7**•8PF_6. The continuous wave (CW) EPR spectra of a solution of **7**•8PF_6 in MeCN (0.20 mM, 0.1 M $TBAPF_6$) were measured (Figure S40) during electrolysis of a 1 ml sample in a glovebox under an atmosphere of argon.

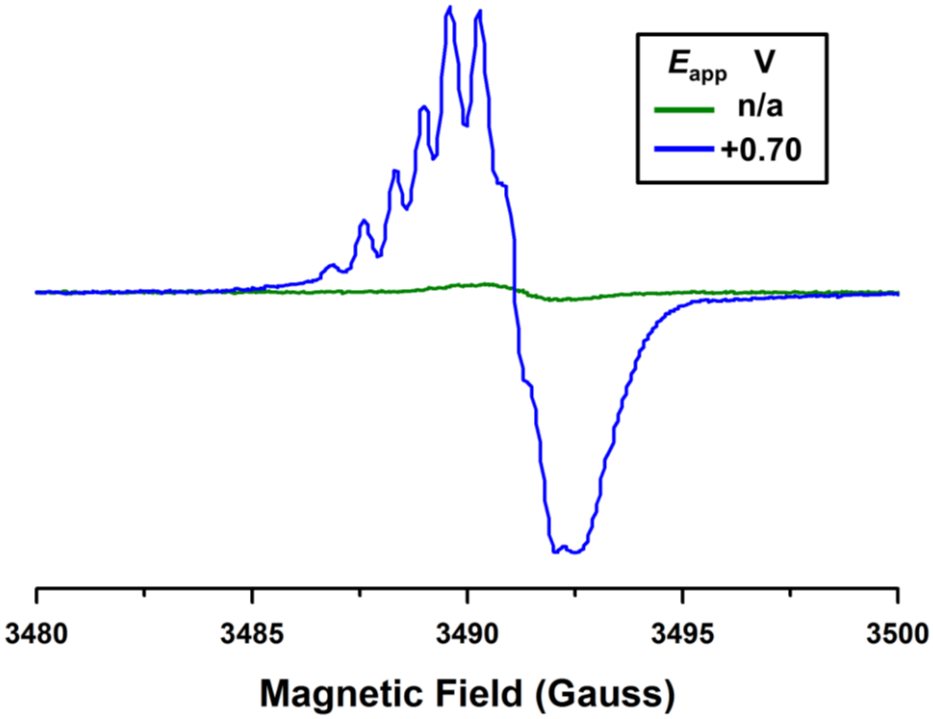


Figure S40. CW EPR Spectra of **7**•8PF_6 (0.20 mM in MeCN, 100 mM $TBAPF_6$, 298 K) recorded before (green curve) and after (blue curve) electrolysis for 30 min at +0.70 V versus Ag/AgCl under argon atmosphere.

The EPR spectrum with no potential being applied confirms the diamagnetic state of $\mathbf{7}^{8+}$. After holding the potential for 30 min at +0.70 V versus Ag/AgCl, a gradual increase in radical signal intensity is observed as a result of the formation of the mixed-valence $(TTF)_2^{\bullet+}$ $\mathbf{7}^{9+}$ state in solution. The spectrum of $\mathbf{7}^{9+}$ displays asymmetric hyperfine splitting, which is indicative of the slow tumbling motion of the radical species.

5) UV-Vis-NIR Spectroscopy

5.1) UV-Vis-NIR spectroscopy of chemically induced switching

The stepwise chemical oxidation of **7**•8PF_6 which was also followed by UV-Vis-NIR spectroscopy, support the observations made from the spectroelectrochemical experiments. The spectroscopic titration of the one-electron oxidizing agent $Fe(ClO_4)_3$ into a 0.15 mM solution of **7**•8PF_6 in MeCN was carried out as shown in Figure S41.

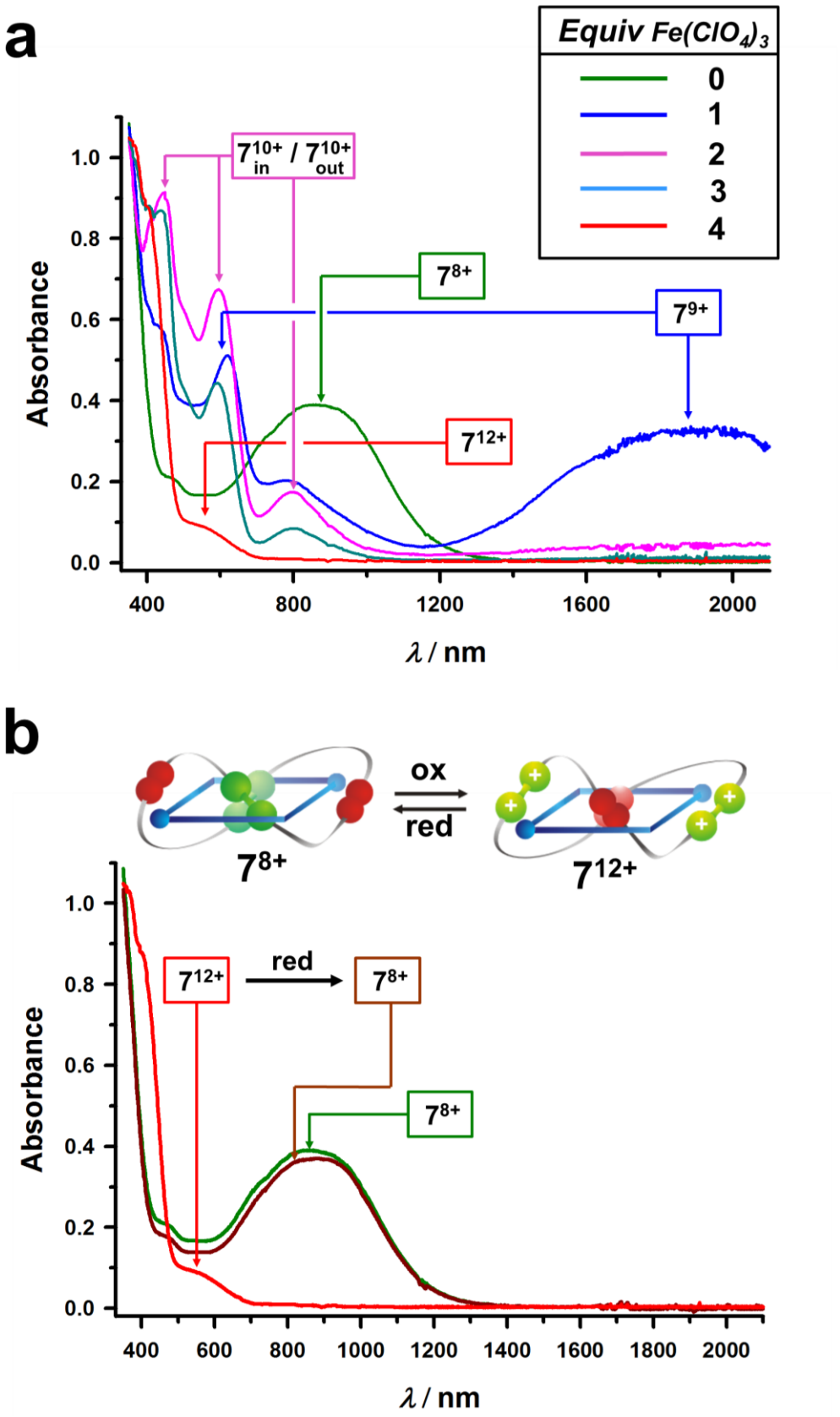


Figure S41. UV-Vis-NIR adsorption spectra of **7**•8PF_6 (0.15 mM in MeCN) recorded (**a**) upon the addition of up to 4.0 equiv of $Fe(ClO_4)_3$. (**b**) The original spectrum is regenerated after treating the solution with Zn dust as reducing agent.

Addition of 1 equiv of oxidant leads to a decrease in the intensity of the charge-transfer band of $\mathbf{7}^{8+}$ and to the appearance of the adsorption band at 620 and 437 nm which are characteristic of the $TTF^{\bullet+}$ radical cation. The formation of the mixed-valence $(TTF)_2^{\bullet+}$ state $\mathbf{7}^{9+}$ is revealed by the appearance of a broad NIR band at 2000 nm. This band disappears after further addition of $Fe(ClO_4)_3$, up to 2 equiv, while the peaks at 620 nm and 437 nm continues to increase. A weak adsorption band at 800 nm was observed, indicating that the formation of a radical-cation dimer $(TTF^{\bullet+})_2$ state occurs only to small extend. The addition of oxidant to generate the fully oxidized $\mathbf{7}^{12+}$ state causes the adsorption bands for the $TTF^{\bullet+}$ radical cation state to disappear and a new band becomes evident at 600 nm, corresponding to the formation of the DNP charge-transfer band.

Zinc dust was added to the solution of **7**•$8PF_6$ in order to reduce the tetrathiafulvalene units from the dicationic state to the neutral form. The solution becomes dark green after a few minutes, an observation which indicates that the original charge-transfer interactions involving the TTF units inside the organoplatinum square were restored. The zinc dust was then filtered off and the UV-Vis spectrum confirmed the presence of charge transfer with an adsorption band center at 860 nm.

5.2) Binding experiments UV-Vis spectroscopy

The binding affinity of the octacationic organoplatinum square $\mathbf{8}^{8+}$ towards the macrocyclic polyether **4** was evaluated (Figure S42) by UV-Vis spectroscopy. The experiments were performed by titrating a solution of **8**•$8PF_6$ into a 1 mM solution of **4** in MeCN at 298 K. The increase of the charge-transfer band, as the ratio of the organoplatinum square $\mathbf{8}^{8+}$ to the macrocyclic polyether **4** is increased, allows a binding constant of 1980 ± 75 L mol^{-1} to be measured between $\mathbf{8}^{8+}$ and **4**.

The adsorption intensity was monitored at 856 nm and the binding constant was calculated using the modified Benesi-Hildebrand equation:

$$(A-A_0)^{-1} = (\Delta\varepsilon[C_G]^{-1})(K_f)^{-1}(C_H)^{-1} + (\Delta\varepsilon[C_G])^{-1}$$

where A_0 is the adsorption of the macrocyclic polyether **4** and A the adsorption of **4** after addition of **8**•$8PF_6$, $\Delta\varepsilon$ is the difference in molar extinction coefficient between **4** and $\mathbf{8}^{8+}$, K_f is the binding constant and C_G and C_H are the concentration of **4** and **8**•$8PF_6$, respectively.

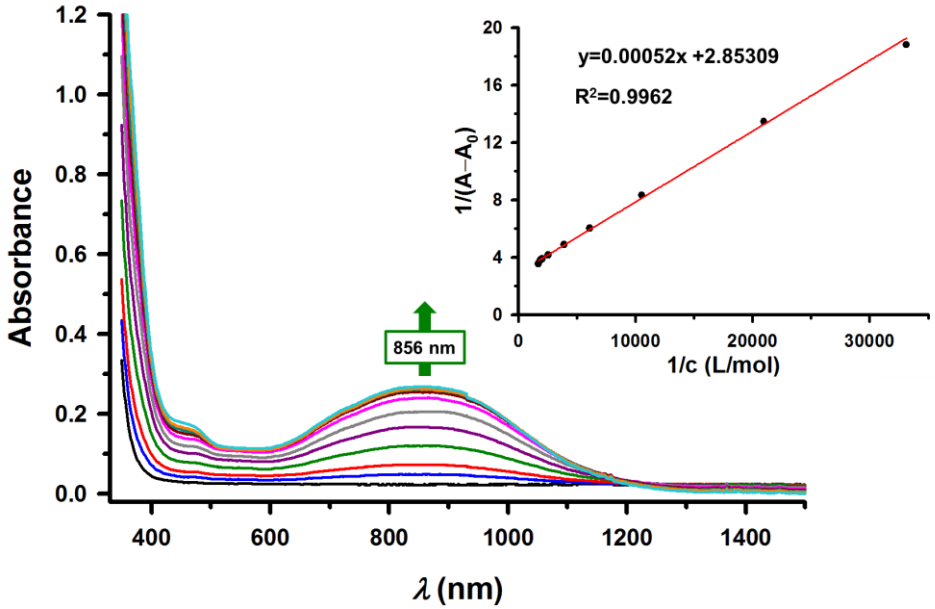


Figure S42. UV-Vis Spectroscopic changes of a 1 mM solution of **4** in MeCN upon addition of increasing amounts of **8**•8PF_6 at 298 K.

The growth of the charge transfer band was monitored at 856 nm and a binding constant of 1980 ± 75 L mol^{-1} was calculated by fitting (Figure S42, inset) the data with the modified Benesi-Hildebrand equation.

F. Computational Analysis

1) Methods

Calculations were performed using density functional theory (DFT) with the M06 functional as implemented in with Jaguar 7.7.[S8] The geometries were optimized in gas phase and then in Poisson-Boltzmann solvation model[S9] for acetonitrile (ε=37.5 and R_0= 2.18 Å) at the level of M06-L/LACVP (S at 6-31G*). The single point energy was refined at the level of M06/LACV3P**++. The total energy is the single point energy and the solvation energy.

2) Calculated coordinates and energies

Energies (Table S1) and atomic coordinates (Table S2) for the co-conformation with both TTF units housed within the cavity of the organoplatinum square (*in* co-conformation) and the state in which both of them leave the cavity (*out* co-conformation) were calculated for different oxidation states of the [3]catenane, $\mathbf{6}^{8+}$, $\mathbf{6}^{9+}$and $\mathbf{6}^{10+}$ and for the molecular Solomon link $\mathbf{7}^{8+}$, $\mathbf{7}^{9+}$and $\mathbf{7}^{10+}$.

Table S1. Calculated energies (in Hartree) for the TTF *in* and *out* co-conformations of the [3]catenane for different oxidation states, $\mathbf{6}^{8+}$, $\mathbf{6}^{9+}$and $\mathbf{6}^{10+}$ and for the molecular Solomon link $\mathbf{7}^{8+}$, $\mathbf{7}^{9+}$and $\mathbf{7}^{10+}$ in the gas phase and in solvent (MeCN).

Molecule	**Solution Phase Energy Solvent MeCN M06-L/LACVP(Hartree)**	**Solution Phase Energy Solvent MeCN M06/LACV3P**++(Hartree)**	**Relative energy (kcal/mol)**
$\mathbf{6}_{in}^{8+}$	-10010.00517	-10009.73852	0
$\mathbf{6}_{out}^{8+}$	-10009.97101	-10009.73619	1.5
$\mathbf{6}_{in}^{9+}$	-10009.80372	-10009.53138	0
$\mathbf{6}_{out}^{9+}$	-10009.79406	-10009.52728	2.6
$\mathbf{6}_{in}^{10+}$	-10009.59736	-10009.29835	11.5
$\mathbf{6}_{out}^{10+}$	-10009.59031	-10009.31662	0

Table S2. Calculated energies (in Hartree) for the TTF *in* and *out* co-conformations of the molecular Solomon link for different oxidation states, $\mathbf{7}^{8+}$, $\mathbf{7}^{9+}$and $\mathbf{7}^{10+}$ in the gas phase and in solvent (MeCN).

Molecule	**Solution Phase Energy Solvent MeCN M06-L/LACVP(Hartree)**	**Solution Phase Energy Solvent MeCN M06/LACV3P**++(Hartree)**	**Relative energy (kcal/mol)**
$\mathbf{7}_{in}^{8+}$	-10010.00442	-10009.74050	0
$\mathbf{7}_{out}^{8+}$	-10009.99722	-10009.74041	2.4
$\mathbf{7}_{in}^{9+}$	-10009.80542	-10009.53000	0
$\mathbf{7}_{out}^{9+}$	-10009.80014	-10009.52143	5.4
$\mathbf{7}_{in}^{10+}$	-10009.56891	-10009.26694	28.7
$\mathbf{7}_{out}^{10+}$	-10009.57175	-10009.31273	0

Table S3. XYZ Calculated coordinates for the TTF *in* and *out* co-conformations of [3]catenane in different oxidation states, $\mathbf{6}^{8+}$, $\mathbf{6}^{9+}$ and $\mathbf{6}^{10+}$.

$\mathbf{6}_{in}^{8+}$	X	Y	Z
Pt1	-6.0912153534	4.9806085560	-0.7418581288
N2	-8.1913590228	4.7524279047	-0.7043462064
H3	-8.5059072662	3.9912509463	-1.3105599461
H4	-8.4875560199	4.5035974581	0.2437396416
N5	-6.5805241667	6.9561143107	-1.1914760349
H6	-5.8743689665	7.5999877309	-0.7963018669
H7	-6.5732664744	7.0922255505	-2.2076590359
N8	-4.0908581445	5.3475291122	-0.7302973781
N9	2.9125678600	5.4715378584	-1.0179758180
N10	4.6388637765	3.8496003658	-0.9367166497
C11	-8.8374707064	6.0553547426	-1.1259457838
H12	-9.8485218608	6.1219436632	-0.7182639689
H13	-8.9098065704	6.0466540381	-2.2166728970
C14	-7.9632476880	7.1987608530	-0.6555528244
H15	-7.8898541818	7.2321395701	0.4360731844
H16	-8.3492718108	8.1608217986	-1.0030396609
C17	-3.4525263890	5.7544872432	-1.8589086930
H18	-4.0686003110	5.9520702742	-2.7274804451
C19	-2.0779961510	5.8905234580	-1.8897639176
H20	-1.6087575830	6.2219131640	-2.8093579805
C21	-1.3151734612	5.6017390648	-0.7414489140
C22	-2.0034553038	5.2524017833	0.4308005026
H23	-1.4935017848	5.0094593549	1.3563000308
C24	-3.3867042566	5.1306974632	0.4106301537
H25	-3.9538022748	4.8600974066	1.2962948541
C26	0.1463224967	5.5842135728	-0.8150054297
C27	0.7785396180	5.4086338088	-2.0577814966
H28	0.2184690338	5.2694924683	-2.9741372178
C29	2.1491762325	5.3519010311	-2.1415972275
H30	2.6675878326	5.1721478173	-3.0740801647
C31	2.3369950896	5.6405675161	0.2130405852
H32	3.0055521787	5.7346700139	1.0599554379
C33	0.9651991632	5.6983018824	0.3313747544
H34	0.5419634561	5.8598670912	1.3146088228
C35	4.3605634746	5.2823301703	-1.1646816399
H36	4.9393096035	5.8883185693	-0.4708064277
H37	4.6572449251	5.5367695947	-2.1823182766
C38	5.1174405837	3.4384540980	0.2693831087
H39	5.3423670326	4.2065719685	0.9990577138
C40	5.3107088760	2.0950091843	0.5174330384
H41	5.7263130886	1.8117614991	1.4758848516
C42	5.0060756705	1.1389729448	-0.4731293609
C43	4.5406731754	1.6080433479	-1.7178216395
H44	4.2987259748	0.9239238894	-2.5210470506
C45	4.3735735552	2.9613816510	-1.9368372014
H46	4.0452434190	3.3859663924	-2.8825403957
N47	-5.6840232950	3.0033255690	-0.3084270065
C48	-5.1941572715	0.2952919111	0.2118622512
C49	-5.2167838540	0.7896805192	-1.1041016541
H50	-5.0359996418	0.1458825943	-1.9574312728
C51	-5.4760497909	2.1316129002	-1.3336159359
H52	-5.5313429309	2.5363010046	-2.3363110865
C53	-5.6086565634	2.5568498815	0.9762007160

H54	-5.7160326786	3.2968805445	1.7648240671
C55	-5.3799722481	1.2161427402	1.2596061361
H56	-5.3972544775	0.9023191477	2.2974729200
Pt57	6.0912153534	-4.9806085560	0.7418581288
N58	8.1913590228	-4.7524279047	0.7043462064
H59	8.5059072662	-3.9912509463	1.3105599461
H60	8.4875560199	-4.5035974581	-0.2437396416
N61	6.5805241667	-6.9561143107	1.1914760349
H62	5.8743689665	-7.5999877309	0.7963018669
H63	6.5732664744	-7.0922255505	2.2076590359
N64	4.0908581445	-5.3475291122	0.7302973781
N65	-2.9125678600	-5.4715378584	1.0179758180
N66	-4.6388637765	-3.8496003658	0.9367166497
C67	8.8374707064	-6.0553547426	1.1259457838
H68	9.8485218608	-6.1219436632	0.7182639689
H69	8.9098065704	-6.0466540381	2.2166728970
C70	7.9632476880	-7.1987608530	0.6555528244
H71	7.8898541818	-7.2321395701	-0.4360731844
H72	8.3492718108	-8.1608217986	1.0030396609
C73	3.4525263890	-5.7544872432	1.8589086930
H74	4.0686003110	-5.9520702742	2.7274804451
C75	2.0779961510	-5.8905234580	1.8897639176
H76	1.6087575830	-6.2219131640	2.8093579805
C77	1.3151734612	-5.6017390648	0.7414489140
C78	2.0034553038	-5.2524017833	-0.4308005026
H79	1.4935017848	-5.0094593549	-1.3563000308
C80	3.3867042566	-5.1306974632	-0.4106301537
H81	3.9538022748	-4.8600974066	-1.2962948541
C82	-0.1463224967	-5.5842135728	0.8150054297
C83	-0.7785396180	-5.4086338088	2.0577814966
H84	-0.2184690338	-5.2694924683	2.9741372178
C85	-2.1491762325	-5.3519010311	2.1415972275
H86	-2.6675878326	-5.1721478173	3.0740801647
C87	-2.3369950896	-5.6405675161	-0.2130405852
H88	-3.0055521787	-5.7346700139	-1.0599554379
C89	-0.9651991632	-5.6983018824	-0.3313747544
H90	-0.5419634561	-5.8598670912	-1.3146088228
C91	-4.3605634746	-5.2823301703	1.1646816399
H92	-4.9393096035	-5.8883185693	0.4708064277
H93	-4.6572449251	-5.5367695947	2.1823182766
C94	-5.1174405837	-3.4384540980	-0.2693831087
H95	-5.3423670326	-4.2065719685	-0.9990577138
C96	-5.3107088760	-2.0950091843	-0.5174330384
H97	-5.7263130886	-1.8117614991	-1.4758848516
C98	-5.0060756705	-1.1389729448	0.4731293609
C99	-4.5406731754	-1.6080433479	1.7178216395
H100	-4.2987259748	-0.9239238894	2.5210470506
C101	-4.3735735552	-2.9613816510	1.9368372014
H102	-4.0452434190	-3.3859663924	2.8825403957
N103	5.6840232950	-3.0033255690	0.3084270065
C104	5.1941572715	-0.2952919111	-0.2118622512
C105	5.2167838540	-0.7896805192	1.1041016541
H106	5.0359996418	-0.1458825943	1.9574312728
C107	5.4760497909	-2.1316129002	1.3336159359
H108	5.5313429309	-2.5363010046	2.3363110865
C109	5.6086565634	-2.5568498815	-0.9762007160
H110	5.7160326786	-3.2968805445	-1.7648240671
C111	5.3799722481	-1.2161427402	-1.2596061361
H112	5.3972544775	-0.9023191477	-2.2974729200
S113	1.0119403597	2.0249713250	-2.7445970235
S114	-1.9418791075	2.3151978410	-2.4312586907

S115	1.3737622697	1.9702296141	0.5358439087
S116	-1.6238437363	1.9020032888	0.7708995918
O117	-2.4967583437	3.6327237758	3.1320373756
O118	-5.1794945727	4.8745466248	3.0064961166
O119	-5.1315172291	7.4346925343	1.5999052280
O120	-4.3095362175	8.7110056071	-0.9128907831
O121	-1.5593577740	9.1444526434	-1.6539524840
O122	4.3267295631	8.3789142787	-0.6058051287
O123	6.7833401809	6.8220371822	-0.4601370195
O124	6.8477600550	4.6650749549	-2.4654327093
O125	4.6163236103	5.1309735927	-4.2765818698
O126	1.9966115353	3.9692243360	-4.8368076761
C127	0.1152480532	2.7164252667	-4.1078306073
C128	-1.2210635008	2.8347319761	-3.9470100256
H129	-1.8931491357	3.2038518185	-4.7153253365
C130	-0.3629999365	2.0471160893	-1.6475406570
C131	-0.2132739295	1.9466516344	-0.2902840756
C132	0.6449982253	2.3636255063	2.0945471916
H133	1.3171976608	2.5795772438	2.9181313692
C134	-0.7027501021	2.3475635532	2.2139931771
C135	-1.4970267378	2.6080551646	3.4475303239
H136	-2.0148697010	1.6931356020	3.7802156773
H137	-0.8437326470	2.9428809272	4.2637969938
C138	-3.3649085294	3.8991454016	4.2827458850
H139	-2.7448659356	4.0505621440	5.1772828621
H140	-4.0214801621	3.0358706054	4.4580283677
C141	-4.1707185974	5.1444107360	4.0311977028
H142	-4.6659772748	5.4449056810	4.9646754909
H143	-3.5197738915	5.9654064176	3.7009583096
C144	-6.2895475509	5.8262199384	2.9907218875
H145	-6.8812868745	5.7159519403	3.9104667375
H146	-6.9005216556	5.5051844714	2.1399043647
C147	-5.8808100072	7.2690202251	2.8388558459
H148	-6.7802346978	7.9026069156	2.8341809841
H149	-5.2594506615	7.5993509588	3.6847514788
C150	-4.5860320878	8.7868628511	1.5042456659
H151	-4.0674700766	9.0360117406	2.4423805893
H152	-5.4015127467	9.5112787250	1.3640697010
C153	-3.6068872153	8.8524615801	0.3670766829
H154	-3.0911043808	9.8194414607	0.3893553145
H155	-2.8559488531	8.0579645053	0.4466488951
C156	-3.8783938534	9.6521885799	-1.9459437886
H157	-3.7474768779	10.6447745815	-1.4965064336
H158	-4.6992977437	9.7032717899	-2.6658502226
C159	-2.6171241212	9.2294947597	-2.6626082869
H160	-2.7328065695	8.2574512212	-3.1557254526
H161	-2.3530873066	9.9768868669	-3.4214064541
C162	-0.2561962947	8.8948480793	-2.0562273873
C163	0.1333798982	8.6970003779	-3.3713867172
H164	-0.5898798023	8.7310257591	-4.1790607493
C165	1.5018305267	8.4928496759	-3.6667076475
H166	1.7967190238	8.3773884635	-4.7055886996
C167	2.4562992073	8.4653468749	-2.6650351218
H168	3.5071872386	8.3226578302	-2.8968657029
C169	2.0702535915	8.6558697069	-1.3095456773
C170	3.0152778589	8.6535750741	-0.2339187036
C171	2.6202609529	8.8831643774	1.0755940865
H172	3.3433484054	8.9056711303	1.8825751507
C173	1.2534907614	9.0879554459	1.3678940155
H174	0.9599866315	9.2606416473	2.3989096539
C175	0.3030766918	9.0751209695	0.3653296306

H176	-0.7442595471	9.2419832043	0.5873067653
C177	0.6942120734	8.8753637393	-0.9850657941
C178	5.3684802296	8.5469664304	0.4214408268
H179	5.1802989464	7.8558661544	1.2528089020
H180	5.3347640936	9.5738385750	0.8021297002
C181	6.6930925867	8.2578917851	-0.2209082771
H182	6.7929534891	8.8029015774	-1.1689289864
H183	7.5028178136	8.5795348971	0.4484548632
C184	8.0049480720	6.4579370191	-1.1680375637
H185	8.8784925708	6.6254906460	-0.5216999945
H186	8.1210972057	7.1002397685	-2.0526765698
C187	7.9335691846	4.9975159305	-1.5449567398
H188	8.8951678930	4.6870066367	-1.9783218569
H189	7.7411788062	4.3850488657	-0.6591365417
C190	6.9996382898	5.2504896269	-3.7955090328
H191	8.0007414038	5.0210470613	-4.1891802021
H192	6.8819329140	6.3413637211	-3.7526002751
C193	5.9476382402	4.6536823073	-4.6935804262
H194	6.1338277254	4.9600039660	-5.7295790509
H195	5.9674614337	3.5585068287	-4.6437991641
C196	3.7312485945	5.5313647333	-5.3740595748
H197	4.3202465267	5.9898050925	-6.1775570941
H198	3.0757147626	6.2995005735	-4.9500023396
C199	2.9006864029	4.3914316184	-5.9103030873
H200	2.3171972385	4.7403832167	-6.7730671289
H201	3.5186504496	3.5422099301	-6.2320346259
C202	0.9213390535	3.0897428801	-5.3058614950
H203	1.3594375768	2.2056732708	-5.7928059898
H204	0.2961708770	3.6077628921	-6.0430014468
S205	-1.0119403597	-2.0249713250	2.7445970235
S206	1.9418791075	-2.3151978410	2.4312586907
S207	-1.3737622697	-1.9702296141	-0.5358439087
S208	1.6238437363	-1.9020032888	-0.7708995918
O209	2.4967583437	-3.6327237758	-3.1320373756
O210	5.1794945727	-4.8745466248	-3.0064961166
O211	5.1315172291	-7.4346925343	-1.5999052280
O212	4.3095362175	-8.7110056071	0.9128907831
O213	1.5593577740	-9.1444526434	1.6539524840
O214	-4.3267295631	-8.3789142787	0.6058051287
O215	-6.7833401809	-6.8220371822	0.4601370195
O216	-6.8477600550	-4.6650749549	2.4654327093
O217	-4.6163236103	-5.1309735927	4.2765818698
O218	-1.9966115353	-3.9692243360	4.8368076761
C219	-0.1152480532	-2.7164252667	4.1078306073
C220	1.2210635008	-2.8347319761	3.9470100256
H221	1.8931491357	-3.2038518185	4.7153253365
C222	0.3629999365	-2.0471160893	1.6475406570
C223	0.2132739295	-1.9466516344	0.2902840756
C224	-0.6449982253	-2.3636255063	-2.0945471916
H225	-1.3171976608	-2.5795772438	-2.9181313692
C226	0.7027501021	-2.3475635532	-2.2139931771
C227	1.4970267378	-2.6080551646	-3.4475303239
H228	2.0148697010	-1.6931356020	-3.7802156773
H229	0.8437326470	-2.9428809272	-4.2637969938
C230	3.3649085294	-3.8991454016	-4.2827458850
H231	2.7448659356	-4.0505621440	-5.1772828621
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C233	4.1707185974	-5.1444107360	-4.0311977028
H234	4.6659772748	-5.4449056810	-4.9646754909
H235	3.5197738915	-5.9654064176	-3.7009583096
C236	6.2895475509	-5.8262199384	-2.9907218875

H237	6.8812868745	-5.7159519403	-3.9104667375
H238	6.9005216556	-5.5051844714	-2.1399043647
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H240	6.7802346978	-7.9026069156	-2.8341809841
H241	5.2594506615	-7.5993509588	-3.6847514788
C242	4.5860320878	-8.7868628511	-1.5042456659
H243	4.0674700766	-9.0360117406	-2.4423805893
H244	5.4015127467	-9.5112787250	-1.3640697010
C245	3.6068872153	-8.8524615801	-0.3670766829
H246	3.0911043808	-9.8194414607	-0.3893553145
H247	2.8559488531	-8.0579645053	-0.4466488951
C248	3.8783938534	-9.6521885799	1.9459437886
H249	3.7474768779	-10.6447745815	1.4965064336
H250	4.6992977437	-9.7032717899	2.6658502226
C251	2.6171241212	-9.2294947597	2.6626082869
H252	2.7328065695	-8.2574512212	3.1557254526
H253	2.3530873066	-9.9768868669	3.4214064541
C254	0.2561962947	-8.8948480793	2.0562273873
C255	-0.1333798982	-8.6970003779	3.3713867172
H256	0.5898798023	-8.7310257591	4.1790607493
C257	-1.5018305267	-8.4928496759	3.6667076475
H258	-1.7967190238	-8.3773884635	4.7055886996
C259	-2.4562992073	-8.4653468749	2.6650351218
H260	-3.5071872386	-8.3226578302	2.8968657029
C261	-2.0702535915	-8.6558697069	1.3095456773
C262	-3.0152778589	-8.6535750741	0.2339187036
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H264	-3.3433484054	-8.9056711303	-1.8825751507
C265	-1.2534907614	-9.0879554459	-1.3678940155
H266	-0.9599866315	-9.2606416473	-2.3989096539
C267	-0.3030766918	-9.0751209695	-0.3653296306
H268	0.7442595471	-9.2419832043	-0.5873067653
C269	-0.6942120734	-8.8753637393	0.9850657941
C270	-5.3684802296	-8.5469664304	-0.4214408268
H271	-5.1802989464	-7.8558661544	-1.2528089020
H272	-5.3347640936	-9.5738385750	-0.8021297002
C273	-6.6930925867	-8.2578917851	0.2209082771
H274	-6.7929534891	-8.8029015774	1.1689289864
H275	-7.5028178136	-8.5795348971	-0.4484548632
C276	-8.0049480720	-6.4579370191	1.1680375637
H277	-8.8784925708	-6.6254906460	0.5216999945
H278	-8.1210972057	-7.1002397685	2.0526765698
C279	-7.9335691846	-4.9975159305	1.5449567398
H280	-8.8951678930	-4.6870066367	1.9783218569
H281	-7.7411788062	-4.3850488657	0.6591365417
C282	-6.9996382898	-5.2504896269	3.7955090328
H283	-8.0007414038	-5.0210470613	4.1891802021
H284	-6.8819329140	-6.3413637211	3.7526002751
C285	-5.9476382402	-4.6536823073	4.6935804262
H286	-6.1338277254	-4.9600039660	5.7295790509
H287	-5.9674614337	-3.5585068287	4.6437991641
C288	-3.7312485945	-5.5313647333	5.3740595748
H289	-4.3202465267	-5.9898050925	6.1775570941
H290	-3.0757147626	-6.2995005735	4.9500023396
C291	-2.9006864029	-4.3914316184	5.9103030873
H292	-2.3171972385	-4.7403832167	6.7730671289
H293	-3.5186504496	-3.5422099301	6.2320346259
C294	-0.9213390535	-3.0897428801	5.3058614950
H295	-1.3594375768	-2.2056732708	5.7928059898
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N5	5.8436166381	3.3501360256	-0.3385903470
C6	-5.4146279472	0.8983880036	0.5144169454
C7	-5.9854152176	1.7874745845	-0.4198519150
C8	-5.6970156478	3.1402899157	-0.3608525641
C9	-4.3063007986	2.7954639017	1.5406583393
C10	-4.5645664342	1.4387339017	1.5006993351
C11	-4.5409309945	5.0758373359	0.6520240926
C12	-2.3706422985	6.0020956973	1.3259890112
C13	-1.0133819532	6.1732647076	1.1550155841
C14	-0.3374851100	5.6114685199	0.0448490446
C15	-1.1422491756	4.9294129989	-0.9068596604
C16	-2.4939600267	4.7850648846	-0.7198451802
C17	1.1230659195	5.6655946759	-0.0863115490
C18	1.9353780973	6.2984412209	0.8845897550
C19	3.3162660337	6.2615402654	0.7833065452
C20	3.1870913393	5.0346044789	-1.2075901168
C21	1.8005333192	5.0451323747	-1.1564911492
C22	7.8456791748	7.6923837025	-0.5048267489
C23	5.6420633364	2.7299343367	-1.5351754586
C24	5.5494848405	1.3462700421	-1.6209918536
C25	5.6475202493	0.5561652096	-0.4609590500
C26	5.8941164118	1.2132102782	0.7591040328
C27	5.9876656094	2.5985940201	0.7888828015
H28	-6.6669607769	1.4411072734	-1.1876927918
H29	-6.1111327627	3.8676738601	-1.0518120220
H30	-3.6520469683	3.2572205824	2.2782494758
H31	-4.0572146689	0.7985067210	2.2126659274
H32	-5.1481736312	5.5940333691	-0.0998675397
H33	-4.7820565950	5.4716610046	1.6421132820
H34	-2.9270221406	6.3942646692	2.1724235811
H35	-0.4916866643	6.7599436245	1.9024043449
H36	-0.7195123101	4.5038859682	-1.8081453802
H37	-3.1280949272	4.2690488193	-1.4317347428
H38	1.5098672591	6.8050937192	1.7417869675
H39	3.9472627179	6.7169311219	1.5358198105
H40	3.7143878901	4.5350659220	-2.0078891208
H41	1.2790308711	4.5207390581	-1.9486744616
H42	8.0006231000	7.5817107947	-1.5802650543
H43	8.1321415349	8.7018202537	-0.1989825029
H44	5.5263266621	3.3737720830	-2.4042433686
H45	5.4077538447	0.8963258769	-2.5967254490
H46	5.9756343741	0.6676513911	1.6924964007
H47	6.1596156614	3.1353346480	1.7132144452
C48	8.6218863057	6.6366266971	0.2439684337
H49	8.4640643271	6.7005309144	1.3232003578
H50	9.6942954256	6.7130517187	0.0475625571
N51	6.3692336621	7.4771957730	-0.2657218580
H52	5.8360010992	7.9695986787	-1.0039179368
H53	6.1056942198	7.8781865254	0.6384242642
N54	8.1028717817	5.2977431393	-0.2179132887
H55	8.4312099822	4.5515722040	0.3993427698
H56	8.4669982687	5.0815615752	-1.1504641806
Pt57	-6.0040388837	-5.4132756743	0.2729629201

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N60	-3.9453769190	-5.6250169281	0.2478066118
N61	-5.8436166381	-3.3501360256	0.3385903470
C62	5.4146279472	-0.8983880036	-0.5144169454
C63	5.9854152176	-1.7874745845	0.4198519150
C64	5.6970156478	-3.1402899157	0.3608525641
C65	4.3063007986	-2.7954639017	-1.5406583393
C66	4.5645664342	-1.4387339017	-1.5006993351
C67	4.5409309945	-5.0758373359	-0.6520240926
C68	2.3706422985	-6.0020956973	-1.3259890112
C69	1.0133819532	-6.1732647076	-1.1550155841
C70	0.3374851100	-5.6114685199	-0.0448490446
C71	1.1422491756	-4.9294129989	0.9068596604
C72	2.4939600267	-4.7850648846	0.7198451802
C73	-1.1230659195	-5.6655946759	0.0863115490
C74	-1.9353780973	-6.2984412209	-0.8845897550
C75	-3.3162660337	-6.2615402654	-0.7833065452
C76	-3.1870913393	-5.0346044789	1.2075901168
C77	-1.8005333192	-5.0451323747	1.1564911492
C78	-7.8456791748	-7.6923837025	0.5048267489
C79	-5.6420633364	-2.7299343367	1.5351754586
C80	-5.5494848405	-1.3462700421	1.6209918536
C81	-5.6475202493	-0.5561652096	0.4609590500
C82	-5.8941164118	-1.2132102782	-0.7591040328
C83	-5.9876656094	-2.5985940201	-0.7888828015
H84	6.6669607769	-1.4411072734	1.1876927918
H85	6.1111327627	-3.8676738601	1.0518120220
H86	3.6520469683	-3.2572205824	-2.2782494758
H87	4.0572146689	-0.7985067210	-2.2126659274
H88	5.1481736312	-5.5940333691	0.0998675397
H89	4.7820565950	-5.4716610046	-1.6421132820
H90	2.9270221406	-6.3942646692	-2.1724235811
H91	0.4916866643	-6.7599436245	-1.9024043449
H92	0.7195123101	-4.5038859682	1.8081453802
H93	3.1280949272	-4.2690488193	1.4317347428
H94	-1.5098672591	-6.8050937192	-1.7417869675
H95	-3.9472627179	-6.7169311219	-1.5358198105
H96	-3.7143878901	-4.5350659220	2.0078891208
H97	-1.2790308711	-4.5207390581	1.9486744616
H98	-8.0006231000	-7.5817107947	1.5802650543
H99	-8.1321415349	-8.7018202537	0.1989825029
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H101	-5.4077538447	-0.8963258769	2.5967254490
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H112	-8.4669982687	-5.0815615752	1.1504641806
S113	-2.5999226583	8.8451081470	-0.2396417779
S114	-2.4925992169	7.4224682059	-2.8381769800
S115	0.7935384088	7.8333792591	-2.9086318337
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O117	-1.1824684023	2.9104963806	2.2397150016
O118	-2.5277816903	4.1260610507	3.5790822937

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C152	6.9002869906	9.0211477325	-3.5581430271
C153	6.2655268733	6.9375275963	-4.6541611788
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C158	2.2065771336	9.2520271553	-1.1266571361
C159	2.2627409609	8.5504646539	-2.2799632500
C160	-0.2302238943	8.4015046823	-1.5840009545
H161	-0.0587004649	0.5534549627	-3.2548693192
H162	-2.1496140722	1.8296464829	0.2894305396
H163	3.3771791614	1.9732365272	-0.2576458243
H164	3.4109456880	2.8976017420	2.0693221651
H165	1.3098768731	3.3299219337	3.2687822385
H166	-4.9930894840	8.4429012787	-0.3240024221
H167	-0.4856401553	4.5321929197	3.3716101599
H168	-0.8861468886	3.0499160293	4.3166993336
H169	-2.4776472946	4.4777281443	5.6541078538
H170	-2.0589143609	5.8828516105	4.6397953937
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H179	-8.6520799748	6.8308877173	-0.6207853571

H180	-7.8076525831	5.6723765813	0.4331838471
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H182	-6.7282509856	8.3543502184	-1.8259370128
H183	-5.3146050476	7.6751143669	-3.8631323863
H184	-5.1406128273	6.0870716164	-3.1478394407
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H186	3.8603397509	9.3797474838	0.2499915866
H187	4.9677267542	11.3324266768	-0.9817263219
H188	3.7663776405	11.1134640969	-2.2760683991
H189	4.8904445870	9.6535365035	-4.1115297652
H190	5.9208471491	10.9121104662	-3.3936894015
H191	7.6423890582	9.2729973709	-2.7958525320
H192	7.3370305353	9.2310152712	-4.5438831573
H193	5.3010543343	7.3259964800	-5.0132825162
H194	7.0214079592	7.1553896858	-5.4225325031
H195	7.0185018725	5.1435149351	-3.7586923357
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H197	2.9765435993	5.4448268380	-4.0810814902
H198	3.9814603509	5.4098987923	-5.5428814926
H199	4.3025279220	2.9008321680	-5.1713660703
H200	2.6244080548	3.3922698092	-5.5249797598
H201	1.6586171428	1.4914174852	-4.2080375311
H202	3.3638460130	0.9352868932	-4.0808055337
H203	3.1763732431	8.4078299289	-2.8464972910
H204	-2.1816174640	0.8981981004	-2.0157320283
S205	2.5999226583	-8.8451081470	0.2396417779
S206	2.4925992169	-7.4224682059	2.8381769800
S207	-0.7935384088	-7.8333792591	2.9086318337
S208	-0.6253549850	-9.3072597707	0.3340893473
O209	1.1824684023	-2.9104963806	-2.2397150016
O210	2.5277816903	-4.1260610507	-3.5790822937
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O212	6.1143313193	-7.3628992758	-1.5141335380
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O214	-2.4023009017	-1.0435514916	2.2924603496
O215	-5.1136366131	-9.5201246377	2.0299185546
O216	-6.6522284938	-7.5887881860	3.4052782093
O217	-4.9765038770	-5.0432183315	3.7093624933
O218	-3.0151124170	-2.9240345382	3.5031090886
C219	-1.1658046889	-1.2995142088	1.6558622165
C220	0.0368421875	-0.9826921319	2.2580726159
C221	1.2427260314	-1.1820397951	1.5496357083
C222	1.2289250756	-1.6989077166	0.2679363451
C223	0.0052076332	-2.0493063347	-0.3541863435
C224	-1.2322460991	-1.8288139326	0.3369237652
C225	-2.4630248222	-2.1429936679	-0.2959604791
C226	-2.4729091174	-2.6624112426	-1.5742079884
C227	-1.2657894018	-2.9159835518	-2.2673279947
C228	-0.0561405344	-2.6350234156	-1.6553899793
C229	4.0869150536	-7.6496598568	2.1171354243
C230	4.1016624384	-8.2804765990	0.9192942979
C231	1.5973388906	-8.2388933808	1.5608531178
C232	1.1762226292	-3.6779779537	-3.4632532693
C233	2.7279109351	-5.0167720425	-4.7325377225
C234	4.1647404322	-5.4554371189	-4.7671537246
C235	5.6188534669	-7.1913889434	-3.8833322026
C236	5.7880718538	-8.1288744095	-2.7173748440
C237	7.3676570580	-7.7293484151	-0.8607424855
C238	7.7069743164	-6.6188470001	0.1049703920
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C240	5.2723562416	-7.1498307714	2.8994514401

C241	-3.3252468514	-10.0157524455	0.4693876353
C242	-4.3057773946	-10.6052664035	1.4663032765
C243	-5.6586480557	-9.8473702621	3.3499736186
C244	-6.9002869906	-9.0211477325	3.5581430271
C245	-6.2655268733	-6.9375275963	4.6541611788
C246	-6.1959272232	-5.4500122189	4.4108312480
C247	-3.8007715260	-4.9207691800	4.5778791902
C248	-3.4420132076	-3.4736450219	4.7956705901
C249	-2.5839723442	-1.5506466167	3.6193325046
C250	-2.2065771336	-9.2520271553	1.1266571361
C251	-2.2627409609	-8.5504646539	2.2799632500
C252	0.2302238943	-8.4015046823	1.5840009545
H253	0.0587004649	-0.5534549627	3.2548693192
H254	2.1496140722	-1.8296464829	-0.2894305396
H255	-3.3771791614	-1.9732365272	0.2576458243
H256	-3.4109456880	-2.8976017420	-2.0693221651
H257	-1.3098768731	-3.3299219337	-3.2687822385
H258	4.9930894840	-8.4429012787	0.3240024221
H259	0.4856401553	-4.5321929197	-3.3716101599
H260	0.8861468886	-3.0499160293	-4.3166993336
H261	2.4776472946	-4.4777281443	-5.6541078538
H262	2.0589143609	-5.8828516105	-4.6397953937
H263	4.3463532626	-5.9770452687	-5.7162634240
H264	4.8475738210	-4.5975571159	-4.7139046707
H265	6.4978405837	-6.5425060782	-3.9917173565
H266	5.4869339760	-7.7608175099	-4.8138131101
H267	6.5816730941	-8.8519613190	-2.9392605917
H268	4.8623252830	-8.6859023420	-2.5297430562
H269	8.1747879976	-7.8264530044	-1.5994405849
H270	7.2575029195	-8.6996877673	-0.3544282204
H271	8.6520799748	-6.8308877173	0.6207853571
H272	7.8076525831	-5.6723765813	-0.4331838471
H273	7.4311222121	-7.1111155721	2.8823106584
H274	6.7282509856	-8.3543502184	1.8259370128
H275	5.3146050476	-7.6751143669	3.8631323863
H276	5.1406128273	-6.0870716164	3.1478394407
H277	-2.9100240603	-10.8400832553	-0.1227878976
H278	-3.8603397509	-9.3797474838	-0.2499915866
H279	-4.9677267542	-11.3324266768	0.9817263219
H280	-3.7663776405	-11.1134640969	2.2760683991
H281	-4.8904445870	-9.6535365035	4.1115297652
H282	-5.9208471491	-10.9121104662	3.3936894015
H283	-7.6423890582	-9.2729973709	2.7958525320
H284	-7.3370305353	-9.2310152712	4.5438831573
H285	-5.3010543343	-7.3259964800	5.0132825162
H286	-7.0214079592	-7.1553896858	5.4225325031
H287	-7.0185018725	-5.1435149351	3.7586923357
H288	-6.2789619997	-4.9040886889	5.3599417164
H289	-2.9765435993	-5.4448268380	4.0810814902
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H291	-4.3025279220	-2.9008321680	5.1713660703
H292	-2.6244080548	-3.3922698092	5.5249797598
H293	-1.6586171428	-1.4914174852	4.2080375311
H294	-3.3638460130	-0.9352868932	4.0808055337
H295	-3.1763732431	-8.4078299289	2.8464972910
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N5	1.2428423879	9.1398699565	1.9714041734
H6	1.7641064709	9.1344933542	1.0917446071
H7	0.3141875812	9.5129388018	1.7553699112
N8	0.5209684659	6.2846857302	1.0172289844
N9	-1.0937378250	3.4150853204	-5.2016967614
N10	-1.2920442025	1.2564724064	-6.1384113374
N11	-1.0249952029	-5.3531951434	-3.6786007369
C12	1.4483546509	9.6558124394	4.3551538118
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H14	0.3791440313	9.8567266736	4.4643680740
C15	1.9377220078	10.0332257380	2.9767055635
H16	1.7349633922	11.0808760197	2.7450618946
H17	3.0125613867	9.8624510077	2.8814988548
C18	-0.7092038697	6.4893328740	0.4753153220
H19	-1.3661539970	7.1628884289	1.0118755253
C20	-1.0894281276	5.8801435683	-0.7148625150
H21	-2.0570458955	6.1323252591	-1.1337364618
C22	-0.1913541298	5.0317732036	-1.3856329150
C23	1.0634393983	4.8124425440	-0.7957883227
H24	1.7948003410	4.1580466521	-1.2549986543
C25	1.3916665173	5.4448651778	0.3929032524
H26	2.3620041848	5.3178837583	0.8566081526
C27	-0.5166287187	4.4577039168	-2.6948877263
C28	-1.8463553114	4.2624661735	-3.1131964257
H29	-2.6794268014	4.5213743164	-2.4706534144
C30	-2.1245446303	3.7348872107	-4.3625939021
H31	-3.1258437516	3.5464852410	-4.7359758453
C32	0.2085011897	3.6134354697	-4.8397194400
H33	0.9690408756	3.3740685889	-5.5716776104
C34	0.5148917213	4.1262989851	-3.5986199529
H35	1.5563271347	4.3119615461	-3.3678462802
C36	-1.3811369803	2.6979975423	-6.4701356347
H37	-2.3796717977	2.9664440735	-6.8198143558
H38	-0.6472097976	2.9720552446	-7.2249851581
C39	-2.3843174327	0.6739989485	-5.5609124429
H40	-3.2656244032	1.2985437825	-5.4583743835
C41	-2.3126858563	-0.6257912524	-5.1009387479
H42	-3.1952104684	-1.0267672575	-4.6158975026
C43	-1.1295887138	-1.3763877970	-5.2376061861
C44	-0.0194547494	-0.7377840590	-5.8399200273
H45	0.9194885181	-1.2559889851	-5.9914624732
C46	-0.1180190044	0.5664040081	-6.2832310646
H47	0.7046482324	1.0833074481	-6.7619235076
C48	-1.0660220262	-2.7636710022	-4.7494806849
C49	-2.2545149236	-3.4917420619	-4.5460512376
H50	-3.2233746392	-3.0857221299	-4.8103539459
C51	-2.2036356251	-4.7689834147	-4.0174845353
H52	-3.1047014034	-5.3449582382	-3.8469191319
C53	0.1446633382	-4.6963929582	-3.9031836011
H54	1.0657571490	-5.2236425178	-3.6595785269
C55	0.1462524688	-3.4066282439	-4.4323568535
H56	1.1031549239	-2.9138902894	-4.5715853664
Pt57	-1.0853044649	-7.2045036363	-2.7819601523
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H59	-1.0745702871	-7.7876998060	-5.2948960505
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H62	-1.7641064709	-9.1344933542	-1.0917446071

H63	-0.3141875812	-9.5129388018	-1.7553699112
N64	-0.5209684659	-6.2846857302	-1.0172289844
N65	1.0937378250	-3.4150853204	5.2016967614
N66	1.2920442025	-1.2564724064	6.1384113374
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C68	-1.4483546509	-9.6558124394	-4.3551538118
H69	-1.9769464283	-10.2103006341	-5.1339191815
H70	-0.3791440313	-9.8567266736	-4.4643680740
C71	-1.9377220078	-10.0332257380	-2.9767055635
H72	-1.7349633922	-11.0808760197	-2.7450618946
H73	-3.0125613867	-9.8624510077	-2.8814988548
C74	0.7092038697	-6.4893328740	-0.4753153220
H75	1.3661539970	-7.1628884289	-1.0118755253
C76	1.0894281276	-5.8801435683	0.7148625150
H77	2.0570458955	-6.1323252591	1.1337364618
C78	0.1913541298	-5.0317732036	1.3856329150
C79	-1.0634393983	-4.8124425440	0.7957883227
H80	-1.7948003410	-4.1580466521	1.2549986543
C81	-1.3916665173	-5.4448651778	-0.3929032524
H82	-2.3620041848	-5.3178837583	-0.8566081526
C83	0.5166287187	-4.4577039168	2.6948877263
C84	1.8463553114	-4.2624661735	3.1131964257
H85	2.6794268014	-4.5213743164	2.4706534144
C86	2.1245446303	-3.7348872107	4.3625939021
H87	3.1258437516	-3.5464852410	4.7359758453
C88	-0.2085011897	-3.6134354697	4.8397194400
H89	-0.9690408756	-3.3740685889	5.5716776104
C90	-0.5148917213	-4.1262989851	3.5986199529
H91	-1.5563271347	-4.3119615461	3.3678462802
C92	1.3811369803	-2.6979975423	6.4701356347
H93	2.3796717977	-2.9664440735	6.8198143558
H94	0.6472097976	-2.9720552446	7.2249851581
C95	2.3843174327	-0.6739989485	5.5609124429
H96	3.2656244032	-1.2985437825	5.4583743835
C97	2.3126858563	0.6257912524	5.1009387479
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C99	1.1295887138	1.3763877970	5.2376061861
C100	0.0194547494	0.7377840590	5.8399200273
H101	-0.9194885181	1.2559889851	5.9914624732
C102	0.1180190044	-0.5664040081	6.2832310646
H103	-0.7046482324	-1.0833074481	6.7619235076
C104	1.0660220262	2.7636710022	4.7494806849
C105	2.2545149236	3.4917420619	4.5460512376
H106	3.2233746392	3.0857221299	4.8103539459
C107	2.2036356251	4.7689834147	4.0174845353
H108	3.1047014034	5.3449582382	3.8469191319
C109	-0.1446633382	4.6963929582	3.9031836011
H110	-1.0657571490	5.2236425178	3.6595785269
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H112	-1.1031549239	2.9138902894	4.5715853664
S113	-1.6765977986	0.9620171494	-1.9773345739
S114	-2.0051232287	-1.8619933358	-1.1074530487
S115	1.4685312021	0.5081983226	-2.4184354556
S116	1.2281919229	-2.2731887895	-1.3133853011
O117	3.1029503645	-4.1590377499	-1.8631611820
O118	2.9105926349	-6.5776218659	-3.6027752084
O119	0.7588295620	-7.1341617669	-5.6371014550
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O121	-2.4066176419	-3.9627566162	-8.0407601476
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O126	-4.4920811597	1.4914128249	-3.3552559846
C127	-3.3104921290	0.4129766856	-1.6182073857
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H129	-4.3867627454	-1.3301424172	-0.9595749928
C130	-0.9186147345	-0.5749419596	-1.6116135873
C131	0.4460249384	-0.7534374025	-1.7314901669
C132	2.8611583293	-0.5648911929	-2.5514922920
H133	3.7551760281	-0.1744483233	-3.0273104440
C134	2.7606593380	-1.8271203882	-2.0616687764
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H137	4.5188905688	-2.7505892628	-1.2176379988
C138	3.9949775856	-5.3319983188	-1.8425246245
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C141	4.1706796973	-5.9612120079	-3.1997543886
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H143	4.4935606924	-5.2303897098	-3.9548756868
C144	3.0887838845	-7.3696566773	-4.8209678745
H145	3.8656314086	-8.1295098506	-4.6491609162
H146	3.4295118840	-6.7243580379	-5.6435762376
C147	1.7853531863	-8.0510915238	-5.1440572157
H148	1.3694874394	-8.4802886050	-4.2253537111
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C150	0.8544023608	-6.8576929153	-7.0715329033
H151	0.7747383369	-7.8020895544	-7.6269934282
H152	1.8180985397	-6.3902343861	-7.3139507815
C153	-0.2756356310	-5.9266586171	-7.4190508555
H154	-0.1744412837	-4.9649371110	-6.9014558755
H155	-0.2802280198	-5.7368092897	-8.4998079184
C156	-2.6520404818	-6.3387721568	-7.9166548696
H157	-3.3527470032	-7.1552571274	-7.7232049376
H158	-2.3124356407	-6.4100485408	-8.9583112366
C159	-3.3544380825	-5.0244729798	-7.6856455674
H160	-4.2445046364	-4.9541215541	-8.3231160507
H161	-3.6586935843	-4.9077277431	-6.6388457116
C162	-2.8673568232	-2.6595857068	-8.1222507784
C163	-4.1496864602	-2.2616269489	-7.7725056404
H164	-4.8750315422	-2.9791510151	-7.4042665984
C165	-4.5278104452	-0.9092554494	-7.9364933092
H166	-5.5464212854	-0.6198098072	-7.6957051668
C167	-3.6366467671	0.0310237862	-8.4259006083
H168	-3.9378649936	1.0639261519	-8.5667586301
C169	-2.3183184307	-0.3619580342	-8.7838790602
C170	-1.9086309336	-1.7242883180	-8.6290614072
C171	-0.5939322237	-2.1187765705	-8.9912050169
H172	-0.3076741998	-3.1575967529	-8.8761064207
C173	0.2880707774	-1.1916204906	-9.5153221622
H174	1.2882068799	-1.4946528017	-9.8101020904
C175	-0.0931231630	0.1581672409	-9.6906672568
H176	0.6134601811	0.8588956550	-10.1206704742
C177	-1.3672616305	0.5624089896	-9.3212866663
C178	-0.9762738306	2.8369439483	-10.1347746477
H179	-0.8037500686	2.4778060831	-11.1552323640
H180	-0.0088668223	2.9325456240	-9.6261398249
C181	-1.7078771555	4.1451794765	-10.1387774565
H182	-1.1845261111	4.8584159927	-10.7907473810
H183	-2.7318081983	4.0190771846	-10.5162096149
C184	-2.4680507430	5.8956873832	-8.6579340068

H185	-3.4092161275	5.8289098859	-9.2225539396
H186	-1.8844119865	6.7220326477	-9.0873890058
C187	-2.7252629204	6.1515954285	-7.1937640066
H188	-1.7877432425	6.2361114353	-6.6377654085
H189	-3.2882744791	7.0886872541	-7.0800406015
C190	-4.7116366374	4.7243561075	-7.1856678416
H191	-4.5211264876	4.1367645618	-8.0940249299
H192	-5.2500437393	5.6408691846	-7.4631288950
C193	-5.5381052240	3.9366451263	-6.2147773820
H194	-5.6331811780	4.4719234838	-5.2607885822
H195	-6.5423934303	3.7742146514	-6.6264329348
C196	-5.8024575992	1.6892098162	-5.3346893591
H197	-5.4286141074	0.6899316820	-5.5803508678
H198	-6.8131436753	1.7901533054	-5.7506665674
C199	-5.8234970929	1.8778942928	-3.8414403431
H200	-6.0404548673	2.9153254518	-3.5548164714
H201	-6.5825430497	1.2288453468	-3.3861294556
C202	-4.4389404664	1.3452804187	-1.9043233184
H203	-5.3738860416	0.9162919045	-1.5242152895
H204	-4.3010111054	2.3297786693	-1.4321988624
S205	1.6765977986	-0.9620171494	1.9773345739
S206	2.0051232287	1.8619933358	1.1074530487
S207	-1.4685312021	-0.5081983226	2.4184354556
S208	-1.2281919229	2.2731887895	1.3133853011
O209	-3.1029503645	4.1590377499	1.8631611820
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O211	-0.7588295620	7.1341617669	5.6371014550
O212	1.5297462126	6.5632802973	7.0155032009
O213	2.4066176419	3.9627566162	8.0407601476
O214	1.8206386912	-1.8717410006	9.4136619179
O215	1.7428978615	-4.6395447102	8.7697261728
O216	3.4459022867	-5.0622502188	6.5367650956
O217	4.8981518234	-2.6310057729	5.9976339083
O218	4.4920811597	-1.4914128249	3.3552559846
C219	3.3104921290	-0.4129766856	1.6182073857
C220	3.4367256170	0.8718032537	1.2121134841
H221	4.3867627454	1.3301424172	0.9595749928
C222	0.9186147345	0.5749419596	1.6116135873
C223	-0.4460249384	0.7534374025	1.7314901669
C224	-2.8611583293	0.5648911929	2.5514922920
H225	-3.7551760281	0.1744483233	3.0273104440
C226	-2.7606593380	1.8271203882	2.0616687764
C227	-3.8115097710	2.8983422707	2.0489936996
H228	-4.3954386816	2.8910434266	2.9776088505
H229	-4.5188905688	2.7505892628	1.2176379988
C230	-3.9949775856	5.3319983188	1.8425246245
H231	-4.9722954790	5.0461080559	1.4331517541
H232	-3.5329214286	6.0447167790	1.1560136146
C233	-4.1706796973	5.9612120079	3.1997543886
H234	-4.9504104441	6.7354409741	3.1347715510
H235	-4.4935606924	5.2303897098	3.9548756868
C236	-3.0887838845	7.3696566773	4.8209678745
H237	-3.8656314086	8.1295098506	4.6491609162
H238	-3.4295118840	6.7243580379	5.6435762376
C239	-1.7853531863	8.0510915238	5.1440572157
H240	-1.3694874394	8.4802886050	4.2253537111
H241	-1.9451272062	8.8566380937	5.8745028088
C242	-0.8544023608	6.8576929153	7.0715329033
H243	-0.7747383369	7.8020895544	7.6269934282
H244	-1.8180985397	6.3902343861	7.3139507815
C245	0.2756356310	5.9266586171	7.4190508555

H246	0.1744412837	4.9649371110	6.9014558755
H247	0.2802280198	5.7368092897	8.4998079184
C248	2.6520404818	6.3387721568	7.9166548696
H249	3.3527470032	7.1552571274	7.7232049376
H250	2.3124356407	6.4100485408	8.9583112366
C251	3.3544380825	5.0244729798	7.6856455674
H252	4.2445046364	4.9541215541	8.3231160507
H253	3.6586935843	4.9077277431	6.6388457116
C254	2.8673568232	2.6595857068	8.1222507784
C255	4.1496864602	2.2616269489	7.7725056404
H256	4.8750315422	2.9791510151	7.4042665984
C257	4.5278104452	0.9092554494	7.9364933092
H258	5.5464212854	0.6198098072	7.6957051668
C259	3.6366467671	-0.0310237862	8.4259006083
H260	3.9378649936	-1.0639261519	8.5667586301
C261	2.3183184307	0.3619580342	8.7838790602
C262	1.9086309336	1.7242883180	8.6290614072
C263	0.5939322237	2.1187765705	8.9912050169
H264	0.3076741998	3.1575967529	8.8761064207
C265	-0.2880707774	1.1916204906	9.5153221622
H266	-1.2882068799	1.4946528017	9.8101020904
C267	0.0931231630	-0.1581672409	9.6906672568
H268	-0.6134601811	-0.8588956550	10.1206704742
C269	1.3672616305	-0.5624089896	9.3212866663
C270	0.9762738306	-2.8369439483	10.1347746477
H271	0.8037500686	-2.4778060831	11.1552323640
H272	0.0088668223	-2.9325456240	9.6261398249
C273	1.7078771555	-4.1451794765	10.1387774565
H274	1.1845261111	-4.8584159927	10.7907473810
H275	2.7318081983	-4.0190771846	10.5162096149
C276	2.4680507430	-5.8956873832	8.6579340068
H277	3.4092161275	-5.8289098859	9.2225539396
H278	1.8844119865	-6.7220326477	9.0873890058
C279	2.7252629204	-6.1515954285	7.1937640066
H280	1.7877432425	-6.2361114353	6.6377654085
H281	3.2882744791	-7.0886872541	7.0800406015
C282	4.7116366374	-4.7243561075	7.1856678416
H283	4.5211264876	-4.1367645618	8.0940249299
H284	5.2500437393	-5.6408691846	7.4631288950
C285	5.5381052240	-3.9366451263	6.2147773820
H286	5.6331811780	-4.4719234838	5.2607885822
H287	6.5423934303	-3.7742146514	6.6264329348
C288	5.8024575992	-1.6892098162	5.3346893591
H289	5.4286141074	-0.6899316820	5.5803508678
H290	6.8131436753	-1.7901533054	5.7506665674
C291	5.8234970929	-1.8778942928	3.8414403431
H292	6.0404548673	-2.9153254518	3.5548164714
H293	6.5825430497	-1.2288453468	3.3861294556
C294	4.4389404664	-1.3452804187	1.9043233184
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N4	3.9594693014	5.5873527908	-0.1890162578
N5	5.8447279213	3.2675190294	-0.2281041758
C6	-5.5293371884	1.0916520212	0.2666767816

C7	-6.0942826900	1.9850738975	-0.6653699054
C8	-5.7721054893	3.3324849372	-0.6205300593
C9	-4.3543452755	2.9681101281	1.2570495705
C10	-4.6434118788	1.6174872531	1.2296141941
C11	-4.5672720724	5.2529522309	0.3721043272
C12	-2.4022123351	6.1264107725	1.1314321483
C13	-1.0354706682	6.2683035956	1.0091888796
C14	-0.3340026586	5.7040636803	-0.0828237366
C15	-1.1197519469	5.0558378453	-1.0731705290
C16	-2.4811320197	4.9402974373	-0.9352544006
C17	1.1343613629	5.7200871607	-0.1557291442
C18	1.9213357773	6.3072694808	0.8626918609
C19	3.3033896494	6.2248565837	0.8243515371
C20	3.2273077218	5.0440391760	-1.1961102885
C21	1.8399367261	5.0999490214	-1.2075234750
C22	7.8883616351	7.5930969013	-0.1842800418
C23	5.6622255312	2.6742429072	-1.4412274555
C24	5.5613344067	1.2927519089	-1.5574512124
C25	5.6418131448	0.4782619919	-0.4133442994
C26	5.8776049025	1.1063918282	0.8236462408
C27	5.9714707021	2.4910239195	0.8849374132
H28	-6.7945783044	1.6480119255	-1.4206886788
H29	-6.1772232861	4.0628453690	-1.3136883933
H30	-3.6786779459	3.4174280110	1.9830367350
H31	-4.1383679085	0.9681934072	1.9367047766
H32	-5.1426915154	5.7745020975	-0.4028308880
H33	-4.8393990998	5.6607332173	1.3500310767
H34	-2.9775800650	6.5175004049	1.9660546291
H35	-0.5280088806	6.8335385777	1.7824936536
H36	-0.6752856319	4.6325474701	-1.9650002388
H37	-3.1022792083	4.4505844735	-1.6767490308
H38	1.4758356406	6.8100210613	1.7114142687
H39	3.9119784378	6.6410084726	1.6171760690
H40	3.7748785901	4.5438370632	-1.9823465777
H41	1.3378231097	4.6122996911	-2.0352313916
H42	8.1092738696	7.5115446604	-1.2506161942
H43	8.1641333619	8.5897217864	0.1691462560
H44	5.5704640467	3.3378839197	-2.2984420488
H45	5.4305680467	0.8618055264	-2.5434699415
H46	5.9498095325	0.5385894731	1.7445551212
H47	6.1309139287	3.0070058877	1.8233014191
C48	8.6044609045	6.5084722174	0.5830604136
H49	8.3773152407	6.5455106253	1.6510951311
H50	9.6876592100	6.5762924125	0.4561624532
N51	6.3967845126	7.3883948672	-0.0444711824
H52	5.9128715428	7.8945642069	-0.8066953833
H53	6.0808162616	7.7777650614	0.8477782094
N54	8.1022353712	5.1876391321	0.0548426297
H55	8.3897944556	4.4230887927	0.6697976325
H56	8.5194849400	4.9915951055	-0.8595483015
Pt57	-6.0902011038	-5.2226932649	0.2654597802
N58	4.7966207022	-3.6872363116	-0.6480569361
N59	3.0234147611	-5.3414103183	-0.5105530423
N60	-4.0237426011	-5.4238220301	0.1636242189
N61	-5.9779509842	-3.1561624040	0.2111848231
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C63	6.0003247642	-1.8982193995	0.3748932399
C64	5.6888824271	-3.2442188468	0.2900109163
C65	4.2137837270	-2.8225823459	-1.5332702691
C66	4.4888821475	-1.4714544703	-1.4594015873
C67	4.4753897329	-5.1345554896	-0.7424665799

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C69	0.8998957647	-6.0674913541	-1.3130788692
C70	0.2617475935	-5.6170487880	-0.1399431955
C71	1.0990384926	-5.0903765864	0.8730389139
C72	2.4562901122	-4.9606513974	0.6765762799
C73	-1.2028811535	-5.6214061159	0.0026704233
C74	-2.0482504539	-6.2233966726	-0.9546809791
C75	-3.4280616727	-6.1096329350	-0.8548713269
C76	-3.2331781290	-4.8433151064	1.1021148069
C77	-1.8456717556	-4.9318399709	1.0479046480
C78	-7.8589202116	-7.5546625359	0.7053603593
C79	-5.8141900135	-2.4957990117	1.3920690016
C80	-5.7280698693	-1.1108602213	1.4359262860
C81	-5.7911272488	-0.3606299889	0.2462575061
C82	-6.0160193679	-1.0553583073	-0.9557417043
C83	-6.1043218348	-2.4432017933	-0.9419508536
H84	6.7234266006	-1.5847289431	1.1187408937
H85	6.1208350900	-3.9891672218	0.9488114044
H86	3.5261494746	-3.2463939680	-2.2639073238
H87	3.9554454429	-0.7993875288	-2.1236617493
H88	5.0584561082	-5.6894657429	0.0036160668
H89	4.7116666681	-5.5117356718	-1.7421179539
H90	2.7940325483	-6.2088599654	-2.3986454600
H91	0.3418854718	-6.5157960912	-2.1263671566
H92	0.7044778284	-4.7667999051	1.8278371215
H93	3.1154893713	-4.5507867309	1.4329152587
H94	-1.6539559849	-6.7805076882	-1.7943591173
H95	-4.0811915349	-6.5542607417	-1.5941723127
H96	-3.7245109375	-4.2964166287	1.8955919561
H97	-1.2971372382	-4.4076989389	1.8218998873
H98	-8.0260677429	-7.4695796102	1.7831952552
H99	-8.1007280226	-8.5767451339	0.4043274504
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H103	-6.2554316164	-3.0109449521	-1.8511512833
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N107	-6.3900120601	-7.2826076214	0.4699634724
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S113	-2.6004918563	9.0095018056	-0.3594004515
S114	-2.4570672367	7.6343401540	-2.9782255482
S115	0.8462162786	7.9679301665	-2.9381236088
S116	0.6244433542	9.3777474235	-0.3368240475
O117	-1.2365320220	2.9958287992	2.0857550989
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O122	2.4771776521	1.0946766913	-2.3280658369
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O126	3.1695961691	2.9656137255	-3.5159750232
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C133	2.4630818080	2.1609308623	0.2778403207
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C144	-5.7975376425	8.3003771176	2.4756149298
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C146	-7.7106352079	6.8324936541	-0.3751835021
C147	-6.5822093813	7.6030827017	-2.4313446373
C148	-5.2422490470	7.4402945762	-3.1221201323
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C150	4.3934930765	10.5709933524	-1.2831069210
C151	5.8204833500	9.8176842653	-3.1141465195
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C153	6.5685163454	6.9259887858	-4.3964828866
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C159	2.3100134593	8.6219755442	-2.2370291081
C160	-0.2072720494	8.5288537395	-1.6384819993
H161	0.0428347236	0.6430723725	-3.3753605823
H162	-2.1513522829	1.9421035032	0.0975589904
H163	3.3940078618	1.9734381354	-0.2398067858
H164	3.3589960203	2.8956362664	2.0860825706
H165	1.2238317779	3.3674578011	3.2079165390
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H167	-0.5536954414	4.6161198973	3.2284261356
H168	-1.0101459319	3.1495667151	4.1716879210
H169	-2.6235660501	4.5659936040	5.4484843509
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H175	-6.5744405212	9.0434749994	2.6897416843
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H181	-7.4011915210	7.4159684335	-3.1358593636
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H184	-5.1179688987	6.3879214887	-3.4147397401
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H187	5.0589516645	11.2620262650	-0.7525604521
H188	3.9079364049	11.1178449418	-2.1020128482
H189	5.1122313403	9.6196472231	-3.9295232023

H190	6.0686223731	10.8859905835	-3.1302347662
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H193	5.6420667717	7.3194946758	-4.8392477401
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H195	7.2259018837	5.1292323760	-3.4325756570
H196	6.6421332553	4.8921496096	-5.0971579674
H197	3.2440709164	5.4839496706	-4.1449402327
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H202	3.4848797531	0.9731826403	-4.0895888804
H203	3.2394243848	8.4705132030	-2.7740589267
H204	-2.1152794525	1.0178185548	-2.2112412910
S205	2.3692772568	-9.0695708526	0.4730555110
S206	3.3293550354	-9.2277693852	3.2507995347
S207	0.5505466316	-10.7641625835	4.1150269724
S208	-0.2866218499	-10.8015774529	1.3059056340
O209	1.0506785565	-2.8196051843	-2.2428305647
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O211	4.1214247474	-6.2327413983	-3.8867759746
O212	5.5550607944	-7.6697828353	-1.8232609265
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C219	-1.3798046812	-1.2566311278	1.6267151481
C220	-0.1897983747	-0.9821278419	2.2733279398
C221	1.0330030408	-1.2001637335	1.5999228588
C222	1.0521871512	-1.6962655266	0.3093668890
C223	-0.1597998969	-1.9904573611	-0.3637139302
C224	-1.4123926873	-1.7463882929	0.2909752747
C225	-2.6290956442	-2.0029204086	-0.3912079559
C226	-2.6142270521	-2.4801950479	-1.6864357999
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C230	4.0013261998	-8.5313690762	0.7891372888
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C238	7.4081630358	-6.8323174531	-0.5452618642
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C252	0.9118204616	-10.3077901067	2.4713659653
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H254	1.9894893547	-1.8385887368	-0.2180057115
H255	-3.5549983318	-1.8121392384	0.1338462869
H256	-3.5416195903	-2.6624773296	-2.2215988391
H257	-1.4211764374	-3.1134798941	-3.3683589606
H258	4.5930400619	-8.1891721504	-0.0647609184
H259	0.3279157597	-4.2684509123	-3.5806223918
H260	0.8315740149	-2.7096207340	-4.3291621974
H261	2.4632911695	-3.9794792721	-5.7672955227
H262	1.8732878024	-5.4813617505	-5.0037501403
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H264	4.7491116533	-4.4243647628	-4.7623116941
H265	6.1167942784	-6.7892787809	-4.2824286644
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H267	5.7062936913	-9.1432464300	-3.3302049026
H268	4.0703218747	-8.6076799239	-2.8959440104
H269	7.5602569094	-7.6803464065	-2.5033941767
H270	7.1705552244	-8.8821815393	-1.2566814305
H271	8.4619725660	-6.9724052060	-0.2733618764
H272	7.2910469495	-5.8174147935	-0.9358024532
H273	7.8505498442	-7.8225018663	2.0126083778
H274	6.9510210741	-8.9326223936	0.9522355800
H275	6.1470397042	-8.8039634892	3.3649678583
H276	5.6809418052	-7.1409345755	3.0904328661
H277	-2.4254292697	-13.2646988357	1.7218146716
H278	-2.8892163181	-11.7571231704	0.9565292887
H279	-4.6596320829	-12.6342459113	2.4518033386
H280	-3.5739084236	-12.5124430576	3.8494028766
H281	-4.8183858630	-9.9705068743	4.8337164780
H282	-5.7075892585	-11.3605650933	4.1929662421
H283	-6.4629485124	-9.8844740781	2.2555009447
H284	-7.1868931817	-9.5416003924	3.8466863692
H285	-5.0317010126	-7.4929436181	4.9461174785
H286	-6.7905722915	-7.7198541442	4.9182119863
H287	-6.9142891415	-5.7716565123	3.2400700754
H288	-6.5259649980	-5.3750592929	4.9279420912
H289	-3.0261160758	-5.3884510200	4.2031086800
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H291	-4.7010641298	-2.9185115162	4.9277166528
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H293	-1.9765126431	-1.3620700553	4.1909733053
H294	-3.6999317727	-0.9154306318	3.9496353524
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H4	2.6666314625	7.9955996509	4.7265237388
N5	1.2305228753	9.1409975989	1.9669782166
H6	1.7338989390	9.1412846469	1.0762922020
H7	0.2934973092	9.5057489271	1.7696250887
N8	0.5223981568	6.2659349753	1.0354247042
N9	-1.0830674398	3.4048146205	-5.1868196141
N10	-1.2820944350	1.2523988686	-6.1385225912
N11	-1.0298740978	-5.3650737056	-3.6935832454

C12	1.4683539022	9.6689849526	4.3453812986
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H14	0.4003246361	9.8670588087	4.4724448874
C15	1.9350990687	10.0437249308	2.9585544331
H16	1.7213774138	11.0884782024	2.7250315164
H17	3.0094370832	9.8806239025	2.8474923050
C18	-0.7122328853	6.4627399149	0.5007508772
H19	-1.3692688450	7.1378178526	1.0343394385
C20	-1.0949785733	5.8546985230	-0.6867718584
H21	-2.0647867387	6.0984772594	-1.1046594517
C22	-0.1925059961	5.0147844064	-1.3614476695
C23	1.0670975966	4.7942319860	-0.7744487443
H24	1.8021867913	4.1444846612	-1.2367695151
C25	1.3943406938	5.4283726925	0.4107455154
H26	2.3708656669	5.3156376793	0.8634505100
C27	-0.5223973422	4.4444195550	-2.6848200480
C28	-1.8459975745	4.2422888649	-3.0969642739
H29	-2.6845152322	4.4907946087	-2.4588572759
C30	-2.1166524477	3.7189926005	-4.3468871430
H31	-3.1158802333	3.5286456994	-4.7251994656
C32	0.2139361029	3.6257631248	-4.8321316351
H33	0.9775754402	3.4127136434	-5.5684307102
C34	0.5134861334	4.1432519778	-3.5928647153
H35	1.5514447067	4.3563066791	-3.3654134752
C36	-1.3721848326	2.6976744162	-6.4582188396
H37	-2.3728623634	2.9693665512	-6.8017891383
H38	-0.6419415422	2.9786243869	-7.2142954460
C39	-2.3722867897	0.6647814747	-5.5610854367
H40	-3.2561416465	1.2881214558	-5.4525654331
C41	-2.3006078221	-0.6379266200	-5.1150356790
H42	-3.1813963746	-1.0466040459	-4.6314976407
C43	-1.1117222485	-1.3871156267	-5.2543977971
C44	-0.0062824471	-0.7422323209	-5.8555958609
H45	0.9363660709	-1.2554523473	-6.0093904822
C46	-0.1080268288	0.5654615559	-6.2884373659
H47	0.7159275764	1.0895932927	-6.7588234789
C48	-1.0523458202	-2.7763563553	-4.7718261808
C49	-2.2468290922	-3.4961580410	-4.5711138281
H50	-3.2135642611	-3.0848819543	-4.8361321393
C51	-2.2077530095	-4.7735403942	-4.0398543655
H52	-3.1120103768	-5.3431178335	-3.8683613842
C53	0.1468312611	-4.7153504457	-3.9209186982
H54	1.0638441403	-5.2482131364	-3.6766152868
C55	0.1567234905	-3.4279689456	-4.4570649761
H56	1.1186274196	-2.9464850007	-4.6030821772
Pt57	-1.0944565977	-7.2080740793	-2.7848582261
N58	-1.6823628108	-8.1902782113	-4.5218763829
H59	-1.1111603109	-7.8025195036	-5.2914070896
H60	-2.6659802790	-7.9956561231	-4.7259873224
N61	-1.2302087776	-9.1412367007	-1.9666166320
H62	-1.7341996156	-9.1412723708	-1.0762479510
H63	-0.2932165309	-9.5058386318	-1.7686263539
N64	-0.5227012695	-6.2659334997	-1.0353402625
N65	1.0833271839	-3.4054857759	5.1867964885
N66	1.2816024134	-1.2525552539	6.1383456138
N67	1.0295182729	5.3649372880	3.6934174206
C68	-1.4680476238	-9.6694155195	-4.3453061273
H69	-2.0099977386	-10.2246842801	-5.1139066176
H70	-0.4001625906	-9.8680332692	-4.4728984924
C71	-1.9350846691	-10.0436015008	-2.9584611842
H72	-1.7232845592	-11.0887846897	-2.7246639714

H73	-3.0091588147	-9.8786976401	-2.8480870621
C74	0.7119177077	-6.4625732613	-0.5006384147
H75	1.3689526629	-7.1377400426	-1.0340559467
C76	1.0948937047	-5.8543673026	0.6866475405
H77	2.0650083442	-6.0978733797	1.1042204932
C78	0.1923919508	-5.0144622807	1.3613390223
C79	-1.0673602850	-4.7942132332	0.7744878365
H80	-1.8023634337	-4.1443407922	1.2367453465
C81	-1.3947239654	-5.4284574040	-0.4106563138
H82	-2.3715344127	-5.3159224234	-0.8628254715
C83	0.5225392689	-4.4441348736	2.6846569324
C84	1.8461480626	-4.2421345500	3.0967110784
H85	2.6845682022	-4.4904101900	2.4583946866
C86	2.1169324123	-3.7194612071	4.3468774709
H87	3.1161790794	-3.5290853922	4.7251851144
C88	-0.2137465901	-3.6259831472	4.8321037088
H89	-0.9771455659	-3.4117599067	5.5683181986
C90	-0.5133290909	-4.1431202559	3.5927100882
H91	-1.5510868859	-4.3565436127	3.3646684649
C92	1.3721086903	-2.6978381830	6.4581155437
H93	2.3728515925	-2.9690993482	6.8018227650
H94	0.6418491729	-2.9789643455	7.2140904162
C95	2.3718739811	-0.6646107323	5.5613493477
H96	3.2558750280	-1.2877974168	5.4529182149
C97	2.3001642344	0.6381289562	5.1154174092
H98	3.1810488321	1.0468502235	4.6320644105
C99	1.1112494317	1.3872306189	5.2547471331
C100	0.0058597218	0.7422254704	5.8559204607
H101	-0.9366982293	1.2555466519	6.0098848569
C102	0.1075621177	-0.5655690285	6.2883793903
H103	-0.7165698719	-1.0896044986	6.7586197988
C104	1.0518096520	2.7764930719	4.7721729867
C105	2.2463718160	3.4961970845	4.5715699404
H106	3.2130567032	3.0849676926	4.8368933755
C107	2.2073331292	4.7734313977	4.0400344401
H108	3.1117150360	5.3429451015	3.8686388659
C109	-0.1473485872	4.7154217392	3.9207111859
H110	-1.0642853406	5.2483858027	3.6761176464
C111	-0.1572272202	3.4281326325	4.4572356781
H112	-1.1190801707	2.9466456938	4.6033476781
S113	-1.8320155587	0.9982937162	-1.9750633224
S114	-2.1091750275	-1.8252481853	-1.1634868248
S115	1.2692803185	0.6165534774	-2.5342194272
S116	1.1234848779	-2.1828792012	-1.4806838949
O117	3.0234580098	-3.9602323590	-1.9286035005
O118	2.8626960224	-6.4773346297	-3.5833484796
O119	0.7322631533	-7.1355837663	-5.6066988127
O120	-1.5502791100	-6.5715771267	-7.0132065149
O121	-2.4251984744	-3.9619895357	-8.0392033797
O122	-1.7910818086	1.8463775999	-9.4322775814
O123	-1.7129253414	4.6123888840	-8.7937018123
O124	-3.4042614328	5.0452130713	-6.5599747277
O125	-4.8837765199	2.6429348896	-6.0170733326
O126	-4.5589919512	1.5611595184	-3.3481411782
C127	-3.4496101263	0.4181126314	-1.6224285627
C128	-3.5558986697	-0.8753911978	-1.2447063361
H129	-4.4931930657	-1.3628724490	-1.0015932865
C130	-1.0539252575	-0.5271328755	-1.6634092201
C131	0.3093509587	-0.6769340651	-1.8322734681
C132	2.7076044012	-0.3825834979	-2.6366105522
H133	3.5908377429	0.0598302947	-3.0839204047

C134	2.6511215243	-1.6523217289	-2.1699258645
C135	3.7220319607	-2.7019243235	-2.1750855403
H136	4.2594989300	-2.7125620435	-3.1311690389
H137	4.4671496266	-2.5268772189	-1.3839124945
C138	3.9041099474	-5.1423491719	-1.8563827975
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C141	4.1077261173	-5.8275541321	-3.1828885882
H142	4.8918798909	-6.5907308916	-3.0656182759
H143	4.4406639114	-5.1304001361	-3.9644733948
C144	3.0642835696	-7.3009037314	-4.7786830235
H145	3.8563669884	-8.0378103219	-4.5831993134
H146	3.3941960524	-6.6704565240	-5.6165723464
C147	1.7784336040	-8.0200415838	-5.0918493637
H148	1.3666649196	-8.4429129531	-4.1683440730
H149	1.9612159840	-8.8346235437	-5.8052829219
C150	0.8372933132	-6.8700763333	-7.0426546007
H151	0.7628488863	-7.8175070734	-7.5926359687
H152	1.8016839936	-6.4023678764	-7.2810942056
C153	-0.2893367041	-5.9403419381	-7.4047048536
H154	-0.1913845059	-4.9773993550	-6.8876777682
H155	-0.2809574975	-5.7544301712	-8.4858434811
C156	-2.6621368936	-6.3455248825	-7.9275418207
H157	-3.3638645401	-7.1633042721	-7.7470557790
H158	-2.3107851540	-6.4090771117	-8.9647603902
C159	-3.3741603189	-5.0371339147	-7.6952540574
H160	-4.2555866266	-4.9623596144	-8.3411080767
H161	-3.6827799447	-4.9207332651	-6.6507289154
C162	-2.8752212938	-2.6698079702	-8.1372349354
C163	-4.1650660524	-2.2621442548	-7.7956161716
H164	-4.8939851080	-2.9756983619	-7.4283432255
C165	-4.5336480428	-0.9174503474	-7.9674667539
H166	-5.5509578356	-0.6193005946	-7.7343069794
C167	-3.6285845590	0.0229271521	-8.4570212419
H168	-3.9290735539	1.0558656032	-8.6008751953
C169	-2.3149662148	-0.3743235499	-8.8020211643
C170	-1.9105792758	-1.7386777509	-8.6450238146
C171	-0.6056130528	-2.1400634991	-9.0103032279
H172	-0.3208866696	-3.1793453676	-8.8964044677
C173	0.2880859493	-1.2155873736	-9.5433475932
H174	1.2838599520	-1.5301756421	-9.8380519647
C175	-0.0799666950	0.1280917916	-9.7176833791
H176	0.6270210734	0.8244015896	-10.1524898496
C177	-1.3571404688	0.5458793529	-9.3419977965
C178	-0.9558907580	2.8195826707	-10.1723206862
H179	-0.8035994393	2.4531508301	-11.1914498339
H180	0.0153104427	2.9127939112	-9.6736989251
C181	-1.6925773648	4.1232495874	-10.1648002504
H182	-1.1756472437	4.8366447591	-10.8210312766
H183	-2.7193039100	3.9973170830	-10.5336384999
C184	-2.4199053524	5.8809155532	-8.6755955949
H185	-3.3611541649	5.8312601429	-9.2409531584
H186	-1.8227501593	6.6988517946	-9.1008891598
C187	-2.6732372706	6.1326547118	-7.2100048045
H188	-1.7352759924	6.2063226895	-6.6535073955
H189	-3.2283061837	7.0732312680	-7.0915222706
C190	-4.6766086006	4.7330711489	-7.2094020871
H191	-4.4982406469	4.1494293138	-8.1222494038
H192	-5.2003889657	5.6594587330	-7.4796628579
C193	-5.5137894590	3.9544454299	-6.2422472661
H194	-5.6104145232	4.4917246806	-5.2898595576

H195	-6.5160542670	3.7967220964	-6.6591800078
C196	-5.8085326303	1.7092807715	-5.3710793307
H197	-5.4258448864	0.7072627548	-5.5887001248
H198	-6.8043967359	1.8022888934	-5.8218998069
C199	-5.8813492462	1.9179254176	-3.8830909663
H200	-6.1259852592	2.9538326414	-3.6159407496
H201	-6.6423528230	1.2601550262	-3.4448530701
C202	-4.5658235622	1.3631741086	-1.9014461959
H203	-5.5153465993	0.9316663013	-1.5672356088
H204	-4.4276731234	2.3269250656	-1.3893179574
S205	1.8320591090	-0.9978525124	1.9754777332
S206	2.1092903230	1.8256870614	1.1638123253
S207	-1.2696815409	-0.6167608727	2.5324439385
S208	-1.1238023157	2.1831685441	1.4807208286
O209	-3.0236857355	3.9596125075	1.9271692600
O210	-2.8597405009	6.4752134388	3.5819813098
O211	-0.7316472579	7.1356366698	5.6067836730
O212	1.5505222838	6.5722179759	7.0139758405
O213	2.4253256993	3.9624549766	8.0394047389
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O215	1.7124011256	-4.6125084879	8.7940060807
O216	3.4041614867	-5.0453055884	6.5602293182
O217	4.8834576013	-2.6430005282	6.0172729608
O218	4.5587435074	-1.5611107968	3.3482548360
C219	3.4496406102	-0.4177687611	1.6226396250
C220	3.5559744191	0.8757133484	1.2447990170
H221	4.4932006422	1.3629765744	1.0010450273
C222	1.0538567424	0.5275347783	1.6634750007
C223	-0.3095229289	0.6771918243	1.8318363726
C224	-2.7078020535	0.3823058620	2.6358041647
H225	-3.5908440704	-0.0600492198	3.0835416517
C226	-2.6514048509	1.6521694165	2.1696346144
C227	-3.7223145681	2.7016617590	2.1749628176
H228	-4.2592345373	2.7128363626	3.1313448834
H229	-4.4680239601	2.5260006044	1.3844291319
C230	-3.9040951658	5.1419088279	1.8554703019
H231	-4.8739964008	4.8566786739	1.4292816150
H232	-3.4119986850	5.8236804824	1.1586272538
C233	-4.1059724930	5.8268712684	3.1821341921
H234	-4.8894498068	6.5908694893	3.0658340858
H235	-4.4390808641	5.1300783753	3.9640061314
C236	-3.0627415111	7.2994845573	4.7769736134
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H238	-3.3932649771	6.6691448613	5.6147080092
C239	-1.7779242394	8.0195759766	5.0914462535
H240	-1.3659578328	8.4431437031	4.1683191141
H241	-1.9619795139	8.8338322152	5.8049463758
C242	-0.8372210892	6.8699339529	7.0426558071
H243	-0.7632313946	7.8172350275	7.5928744139
H244	-1.8016330129	6.4020271206	7.2806851622
C245	0.2896563335	5.9405727493	7.4049698516
H246	0.1918015660	4.9775724403	6.8879596522
H247	0.2811106712	5.7546319530	8.4860652148
C248	2.6621000410	6.3463451037	7.9291313510
H249	3.3631271524	7.1654639395	7.7514083090
H250	2.3097379959	6.4088302434	8.9660317780
C251	3.3744400383	5.0382553414	7.6960749112
H252	4.2558801314	4.9632506250	8.3418105522
H253	3.6830295641	4.9219916910	6.6515420229
C254	2.8750514985	2.6703524108	8.1373516974
C255	4.1648992624	2.2623987280	7.7957851545

H256	4.8939162945	2.9760293988	7.4289904015
C257	4.5334137032	0.9177266296	7.9676701499
H258	5.5509080036	0.6198811549	7.7349591989
C259	3.6282456400	-0.0227224389	8.4571212490
H260	3.9286322510	-1.0557067242	8.6009549626
C261	2.3146329610	0.3746290689	8.8020393040
C262	1.9103435182	1.7390759265	8.6450528393
C263	0.6054400043	2.1404446726	9.0105218496
H264	0.3207700644	3.1797432944	8.8966500552
C265	-0.2883427466	1.2160493826	9.5436736877
H266	-1.2839399333	1.5308574457	9.8386059602
C267	0.0795429146	-0.1277285879	9.7177604391
H268	-0.6276845487	-0.8242512325	10.1518880183
C269	1.3567338622	-0.5455452895	9.3420493553
C270	0.9557509021	-2.8193754279	10.1725102544
H271	0.8038260887	-2.4532949357	11.1919386943
H272	-0.0155282297	-2.9126120476	9.6740431729
C273	1.6923770464	-4.1231241746	10.1650121821
H274	1.1756426336	-4.8363878118	10.8215228974
H275	2.7191398702	-3.9969403299	10.5336628016
C276	2.4193666742	-5.8809662871	8.6757744806
H277	3.3606210228	-5.8314912850	9.2411492447
H278	1.8222672486	-6.6990931626	9.1008168166
C279	2.6730104101	-6.1326234918	7.2102243114
H280	1.7352164499	-6.2064084704	6.6534670623
H281	3.2280576811	-7.0733136111	7.0922363209
C282	4.6765401653	-4.7330952764	7.2096762751
H283	4.4981631759	-4.1493953371	8.1224784422
H284	5.2002447885	-5.6595225282	7.4799194124
C285	5.5136227144	-3.9543866830	6.2424840113
H286	5.6103569235	-4.4916067918	5.2900556571
H287	6.5159346945	-3.7966019545	6.6592937417
C288	5.8082382450	-1.7092826631	5.3713090566
H289	5.4256936234	-0.7072453674	5.5890271484
H290	6.8040993649	-1.8025173815	5.8220751388
C291	5.8810641052	-1.9179151009	3.8833363367
H292	6.1257095358	-2.9538002210	3.6161092969
H293	6.6421913991	-1.2601697766	3.4452402521
C294	4.5657025381	-1.3630169397	1.9016247903
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N4	4.1604408815	5.2991122752	0.0016447158
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C6	-5.5528546404	1.1305225886	0.1573014591
C7	-6.1041811208	2.0739963069	-0.7328958695
C8	-5.7099518065	3.4002808127	-0.6740175246
C9	-4.2502281411	2.9218414838	1.1453172395
C10	-4.6066197620	1.5885967339	1.0984592219
C11	-4.3963516077	5.2374478969	0.3400311261
C12	-2.2079012991	5.8187799533	1.3008055962
C13	-0.8284551469	5.9073956483	1.2281432641
C14	-0.1295692611	5.5109285037	0.0695438915
C15	-0.9145636876	5.1040486789	-1.0367460724
C16	-2.2882842854	5.0346325432	-0.9435005683

C17	1.3474519294	5.4762885840	0.0234848257
C18	2.1279152057	5.9791917493	1.0857194283
C19	3.5099958430	5.8743598068	1.0526651458
C20	3.4313461713	4.8100980743	-1.0340274599
C21	2.0425303862	4.8855287965	-1.0474873703
C22	7.8954977010	7.5800948452	-0.3488441814
C23	5.9938568892	2.4610035023	-1.2133730360
C24	5.8642290044	1.0802244444	-1.2852509224
C25	5.8813551079	0.3074803177	-0.1084716801
C26	6.1081540368	0.9710557584	1.1105810464
C27	6.2300076805	2.3563729446	1.1258372342
H28	-6.8477545038	1.7912382907	-1.4687245153
H29	-6.0997582248	4.1549053256	-1.3470685445
H30	-3.5414415683	3.3099682041	1.8752048295
H31	-4.1065565480	0.8959310451	1.7700414185
H32	-4.8903283930	5.8029057838	-0.4586820837
H33	-4.6925787390	5.6558581420	1.3075728158
H34	-2.7835547767	6.0590239704	2.1955117486
H35	-0.3124581865	6.2718539757	2.1077996661
H36	-0.4674350794	4.8395774970	-1.9865252753
H37	-2.9113044717	4.7207434547	-1.7711508850
H38	1.6847041664	6.4620864688	1.9473992381
H39	4.1203648001	6.2451366927	1.8656136690
H40	3.9776953024	4.3579413292	-1.8500595546
H41	1.5342011276	4.4475014180	-1.8989689991
H42	8.0847758347	7.5178636653	-1.4253366029
H43	8.0908263946	8.6074581465	-0.0317158846
H44	5.9517821665	3.0986014354	-2.0917489728
H45	5.7495600778	0.6115360069	-2.2557249309
H46	6.1416835710	0.4340959992	2.0521692571
H47	6.3732456958	2.9012646233	2.0500579545
C48	8.7556159201	6.5966740397	0.4089390590
H49	8.6132702128	6.6919547454	1.4876159724
H50	9.8165434866	6.7370525938	0.1879065684
N51	6.4405204700	7.2398897889	-0.1313051864
H52	5.8981255244	7.5745045669	-0.9530122575
H53	6.0906024430	7.6951355987	0.7155697952
N54	8.3263814381	5.2011695791	0.0172630409
H55	8.7107198958	4.5166457518	0.6734159879
H56	8.7029577294	4.9572225810	-0.9040693971
Pt57	-6.2278330742	-5.1644014939	0.0127981955
N58	4.7881036781	-3.8051494440	-0.2517374185
N59	2.9228631206	-5.3653069482	-0.2257464379
N60	-4.1604408815	-5.2991122752	-0.0016447158
N61	-6.1457164487	-3.0935341658	0.0159745320
C62	5.5528546404	-1.1305225886	-0.1573014591
C63	6.1041811208	-2.0739963069	0.7328958695
C64	5.7099518065	-3.4002808127	0.6740175246
C65	4.2502281411	-2.9218414838	-1.1453172395
C66	4.6066197620	-1.5885967339	-1.0984592219
C67	4.3963516077	-5.2374478969	-0.3400311261
C68	2.2079012991	-5.8187799533	-1.3008055962
C69	0.8284551469	-5.9073956483	-1.2281432641
C70	0.1295692611	-5.5109285037	-0.0695438915
C71	0.9145636876	-5.1040486789	1.0367460724
C72	2.2882842854	-5.0346325432	0.9435005683
C73	-1.3474519294	-5.4762885840	-0.0234848257
C74	-2.1279152057	-5.9791917493	-1.0857194283
C75	-3.5099958430	-5.8743598068	-1.0526651458
C76	-3.4313461713	-4.8100980743	1.0340274599
C77	-2.0425303862	-4.8855287965	1.0474873703

C78	-7.8954977010	-7.5800948452	0.3488441814
C79	-5.9938568892	-2.4610035023	1.2133730360
C80	-5.8642290044	-1.0802244444	1.2852509224
C81	-5.8813551079	-0.3074803177	0.1084716801
C82	-6.1081540368	-0.9710557584	-1.1105810464
C83	-6.2300076805	-2.3563729446	-1.1258372342
H84	6.8477545038	-1.7912382907	1.4687245153
H85	6.0997582248	-4.1549053256	1.3470685445
H86	3.5414415683	-3.3099682041	-1.8752048295
H87	4.1065565480	-0.8959310451	-1.7700414185
H88	4.8903283930	-5.8029057838	0.4586820837
H89	4.6925787390	-5.6558581420	-1.3075728158
H90	2.7835547767	-6.0590239704	-2.1955117486
H91	0.3124581865	-6.2718539757	-2.1077996661
H92	0.4674350794	-4.8395774970	1.9865252753
H93	2.9113044717	-4.7207434547	1.7711508850
H94	-1.6847041664	-6.4620864688	-1.9473992381
H95	-4.1203648001	-6.2451366927	-1.8656136690
H96	-3.9776953024	-4.3579413292	1.8500595546
H97	-1.5342011276	-4.4475014180	1.8989689991
H98	-8.0847758347	-7.5178636653	1.4253366029
H99	-8.0908263946	-8.6074581465	0.0317158846
H100	-5.9517821665	-3.0986014354	2.0917489728
H101	-5.7495600778	-0.6115360069	2.2557249309
H102	-6.1416835710	-0.4340959992	-2.0521692571
H103	-6.3732456958	-2.9012646233	-2.0500579545
C104	-8.7556159201	-6.5966740397	-0.4089390590
H105	-8.6132702128	-6.6919547454	-1.4876159724
H106	-9.8165434866	-6.7370525938	-0.1879065684
N107	-6.4405204700	-7.2398897889	0.1313051864
H108	-5.8981255244	-7.5745045669	0.9530122575
H109	-6.0906024430	-7.6951355987	-0.7155697952
N110	-8.3263814381	-5.2011695791	-0.0172630409
H111	-8.7107198958	-4.5166457518	-0.6734159879
H112	-8.7029577294	-4.9572225810	0.9040693971
S113	-2.1988896566	9.6330457775	-0.8964512183
S114	-3.4122627942	10.0943866130	-3.5234832159
S115	-0.8862937877	11.9050287373	-4.4278515919
S116	0.4275577421	11.4534711951	-1.8469997761
O117	-1.1019762174	2.6830566634	2.0182237337
O118	-2.5072357221	3.7151638411	3.4477764798
O119	-4.0723628956	6.1085377830	3.6269763494
O120	-5.1613765312	7.8153441071	1.5891446897
O121	-6.3477320208	7.3418689357	-0.9265913954
O122	2.8329846551	0.9820691087	-2.2796955245
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O124	5.5455202262	8.2272001628	-2.6561161542
O125	5.3397619391	5.1530580107	-3.3627739780
O126	3.5598275540	2.8718896119	-3.4235249653
C127	1.5484798250	1.2432534994	-1.7574869058
C128	0.3971800243	1.0364915111	-2.4967805926
C129	-0.8607108841	1.2705021078	-1.9001517041
C130	-0.9568433816	1.7038163746	-0.5903690009
C131	0.2128828467	1.9204892503	0.1802372905
C132	1.5010086072	1.6731105606	-0.4011120245
C133	2.6749949869	1.8710192115	0.3701372385
C134	2.5840007228	2.2770777913	1.6858474042
C135	1.3278813910	2.5322346048	2.2815510963
C136	0.1738136112	2.3857954491	1.5306750401
C137	-4.3689757322	9.1787988036	-2.3727171159
C138	-3.7815563613	8.9639728485	-1.1648725329

C139	-2.0463601709	10.3596051101	-2.4729222802
C140	-1.1828456976	3.1908723929	3.3691327776
C141	-2.7630359475	4.4039471733	4.7225123206
C142	-4.1122997037	5.0600077674	4.6466809645
C143	-4.8680241127	7.2923338117	3.9621321631
C144	-4.6414485449	8.3043981248	2.8694496279
C145	-6.5830879594	8.1254790259	1.4017002391
C146	-7.1143137727	7.2237907261	0.3156450441
C147	-6.7255168454	8.5384434491	-1.6912595934
C148	-5.7356547405	8.7345247147	-2.8205682628
C149	2.6049222674	13.0670044905	-2.6154309740
C150	3.7729775294	12.4757646099	-3.3961894786
C151	5.2541052484	10.5898535190	-3.5382471598
C152	5.9864842956	9.6320202514	-2.6205082207
C153	5.9186944093	7.5503937288	-3.9109858367
C154	6.3840877404	6.1284422000	-3.6750608255
C155	4.4367357135	4.8645034518	-4.4833038003
C156	4.2442010928	3.3771193187	-4.6240074906
C157	3.1588537179	1.4933251226	-3.5799844590
C158	1.2717448567	12.4773701909	-2.9832859196
C159	0.6327432669	12.6760168227	-4.1693471634
C160	-0.9503862284	11.1388689160	-2.8646462504
H161	0.4521098421	0.6869755616	-3.5232784299
H162	-1.9252343450	1.8570806214	-0.1257993586
H163	3.6311178246	1.6936282700	-0.1029116333
H164	3.4777419088	2.4112392795	2.2886901908
H165	1.2946318066	2.8375404577	3.3214174089
H166	-4.2585915424	8.4376990861	-0.3361628136
H167	-0.4408281274	3.9891007407	3.5274799493
H168	-1.0201016998	2.3799469963	4.0923798178
H169	-2.7341812437	3.6762375772	5.5421493830
H170	-1.9780368649	5.1538888240	4.8848521864
H171	-4.3424923973	5.5006050880	5.6241823735
H172	-4.9005035654	4.3393207639	4.4002167910
H173	-5.9276866602	7.0154836391	4.0448715020
H174	-4.5396248485	7.6922389743	4.9301928821
H175	-5.1070754262	9.2634127899	3.1261527491
H176	-3.5723554248	8.4718086497	2.7136358550
H177	-7.1408208568	7.9427214583	2.3295797039
H178	-6.6826838696	9.1902457511	1.1534005183
H179	-8.1739602010	7.4393950297	0.1269985570
H180	-7.0341120765	6.1740141548	0.6118492681
H181	-7.7355319056	8.3961048658	-2.0945177651
H182	-6.7378165033	9.4149850449	-1.0304671287
H183	-6.1548271000	9.4779236407	-3.5092277863
H184	-5.6552436215	7.8073543611	-3.3999926989
H185	2.5709964676	14.1438017679	-2.8201861397
H186	2.8022772438	12.9624355230	-1.5443663912
H187	4.6535720419	13.1236399922	-3.2765405306
H188	3.5402556486	12.4222597348	-4.4695881384
H189	4.9665855001	10.1168834802	-4.4869669239
H190	5.9401077892	11.4152675571	-3.7795415405
H191	5.8544995302	9.9500772105	-1.5842442809
H192	7.0584302549	9.6553005536	-2.8635753330
H193	5.0745459517	7.5813646514	-4.6058939633
H194	6.7466127764	8.1037094485	-4.3745454380
H195	7.0640518632	6.0818170775	-2.8178644989
H196	6.9324718672	5.7925118848	-4.5665345289
H197	3.4780813780	5.3694953981	-4.3088808922
H198	4.8632094974	5.2508339639	-5.4174278928
H199	5.2053933545	2.8560272445	-4.7357196073

H200	3.6309688777	3.1735194278	-5.5122338477
H201	2.3092011373	1.4214907035	-4.2701736807
H202	3.9916467167	0.8817609098	-3.9431313204
H203	1.0124666296	13.3015728992	-4.9698576802
H204	-1.7575273391	1.0857589068	-2.4829440022
S205	2.1988896566	-9.6330457775	0.8964512183
S206	3.4122627942	-10.0943866130	3.5234832159
S207	0.8862937877	-11.9050287373	4.4278515919
S208	-0.4275577421	-11.4534711951	1.8469997761
O209	1.1019762174	-2.6830566634	-2.0182237337
O210	2.5072357221	-3.7151638411	-3.4477764798
O211	4.0723628956	-6.1085377830	-3.6269763494
O212	5.1613765312	-7.8153441071	-1.5891446897
O213	6.3477320208	-7.3418689357	0.9265913954
O214	-2.8329846551	-0.9820691087	2.2796955245
O215	-4.0730004210	-11.1462769686	2.8755743121
O216	-5.5455202262	-8.2272001628	2.6561161542
O217	-5.3397619391	-5.1530580107	3.3627739780
O218	-3.5598275540	-2.8718896119	3.4235249653
C219	-1.5484798250	-1.2432534994	1.7574869058
C220	-0.3971800243	-1.0364915111	2.4967805926
C221	0.8607108841	-1.2705021078	1.9001517041
C222	0.9568433816	-1.7038163746	0.5903690009
C223	-0.2128828467	-1.9204892503	-0.1802372905
C224	-1.5010086072	-1.6731105606	0.4011120245
C225	-2.6749949869	-1.8710192115	-0.3701372385
C226	-2.5840007228	-2.2770777913	-1.6858474042
C227	-1.3278813910	-2.5322346048	-2.2815510963
C228	-0.1738136112	-2.3857954491	-1.5306750401
C229	4.3689757322	-9.1787988036	2.3727171159
C230	3.7815563613	-8.9639728485	1.1648725329
C231	2.0463601709	-10.3596051101	2.4729222802
C232	1.1828456976	-3.1908723929	-3.3691327776
C233	2.7630359475	-4.4039471733	-4.7225123206
C234	4.1122997037	-5.0600077674	-4.6466809645
C235	4.8680241127	-7.2923338117	-3.9621321631
C236	4.6414485449	-8.3043981248	-2.8694496279
C237	6.5830879594	-8.1254790259	-1.4017002391
C238	7.1143137727	-7.2237907261	-0.3156450441
C239	6.7255168454	-8.5384434491	1.6912595934
C240	5.7356547405	-8.7345247147	2.8205682628
C241	-2.6049222674	-13.0670044905	2.6154309740
C242	-3.7729775294	-12.4757646099	3.3961894786
C243	-5.2541052484	-10.5898535190	3.5382471598
C244	-5.9864842956	-9.6320202514	2.6205082207
C245	-5.9186944093	-7.5503937288	3.9109858367
C246	-6.3840877404	-6.1284422000	3.6750608255
C247	-4.4367357135	-4.8645034518	4.4833038003
C248	-4.2442010928	-3.3771193187	4.6240074906
C249	-3.1588537179	-1.4933251226	3.5799844590
C250	-1.2717448567	-12.4773701909	2.9832859196
C251	-0.6327432669	-12.6760168227	4.1693471634
C252	0.9503862284	-11.1388689160	2.8646462504
H253	-0.4521098421	-0.6869755616	3.5232784299
H254	1.9252343450	-1.8570806214	0.1257993586
H255	-3.6311178246	-1.6936282700	0.1029116333
H256	-3.4777419088	-2.4112392795	-2.2886901908
H257	-1.2946318066	-2.8375404577	-3.3214174089
H258	4.2585915424	-8.4376990861	0.3361628136
H259	0.4408281274	-3.9891007407	-3.5274799493
H260	1.0201016998	-2.3799469963	-4.0923798178

H261	2.7341812437	-3.6762375772	-5.5421493830
H262	1.9780368649	-5.1538888240	-4.8848521864
H263	4.3424923973	-5.5006050880	-5.6241823735
H264	4.9005035654	-4.3393207639	-4.4002167910
H265	5.9276866602	-7.0154836391	-4.0448715020
H266	4.5396248485	-7.6922389743	-4.9301928821
H267	5.1070754262	-9.2634127899	-3.1261527491
H268	3.5723554248	-8.4718086497	-2.7136358550
H269	7.1408208568	-7.9427214583	-2.3295797039
H270	6.6826838696	-9.1902457511	-1.1534005183
H271	8.1739602010	-7.4393950297	-0.1269985570
H272	7.0341120765	-6.1740141548	-0.6118492681
H273	7.7355319056	-8.3961048658	2.0945177651
H274	6.7378165033	-9.4149850449	1.0304671287
H275	6.1548271000	-9.4779236407	3.5092277863
H276	5.6552436215	-7.8073543611	3.3999926989
H277	-2.5709964676	-14.1438017679	2.8201861397
H278	-2.8022772438	-12.9624355230	1.5443663912
H279	-4.6535720419	-13.1236399922	3.2765405306
H280	-3.5402556486	-12.4222597348	4.4695881384
H281	-4.9665855001	-10.1168834802	4.4869669239
H282	-5.9401077892	-11.4152675571	3.7795415405
H283	-5.8544995302	-9.9500772105	1.5842442809
H284	-7.0584302549	-9.6553005536	2.8635753330
H285	-5.0745459517	-7.5813646514	4.6058939633
H286	-6.7466127764	-8.1037094485	4.3745454380
H287	-7.0640518632	-6.0818170775	2.8178644989
H288	-6.9324718672	-5.7925118848	4.5665345289
H289	-3.4780813780	-5.3694953981	4.3088808922
H290	-4.8632094974	-5.2508339639	5.4174278928
H291	-5.2053933545	-2.8560272445	4.7357196073
H292	-3.6309688777	-3.1735194278	5.5122338477
H293	-2.3092011373	-1.4214907035	4.2701736807
H294	-3.9916467167	-0.8817609098	3.9431313204
H295	-1.0124666296	-13.3015728992	4.9698576802
H296	1.7575273391	-1.0857589068	2.4829440022

Table S4. XYZ Calculated coordinates for the TTF *in* and *out* co-conformations of molecular Solomon link in different oxidation states, $\mathbf{7}^{8+}$, $\mathbf{7}^{9+}$ and $\mathbf{7}^{10+}$.

$\mathbf{7}_{in}^{8+}$	X	Y	Z
Pt1	4.0025855599	18.5300354183	19.0781240662
Pt2	10.1776710097	5.6062362559	25.3509703117
N3	5.9309844248	17.8673502007	19.3785852824
N4	12.3839805211	15.0575020096	20.0720563401
N5	13.1698411820	13.0153991539	20.9998854239
N6	10.8792394713	7.2663080293	24.3640074685
N7	8.2944560134	6.0707013946	24.6470200946
N8	2.0487623552	8.0504129120	21.9954173003
N9	1.1952266989	10.0664211625	21.0484242962
N10	3.3198745419	16.6199371741	19.4641518314
C11	2.1396383861	20.7627574018	18.5355727988
C12	3.4612260660	21.2044389374	17.9484034917
C13	6.4921056953	17.1498156011	18.3644112197
C14	7.7728715960	16.6356605428	18.4707068537

C15	8.5322756450	16.8285540688	19.6429440988
C16	7.9274527656	17.5814802134	20.6743304483
C17	6.6450016122	18.0848314261	20.5154517633
C18	9.8704652842	16.2481131183	19.7861556214
C19	10.4628846515	15.5018261765	18.7385792624
C20	11.6989943093	14.9177977516	18.8954731600
C21	11.8639861825	15.7950347070	21.1025472471
C22	10.6247990295	16.3859546897	20.9742932105
C23	13.5978386286	14.2552265354	20.3131034453
C24	13.1770711617	12.9834703438	22.3649372584
C25	12.7159754501	11.8589978712	23.0268290201
C26	12.2474941724	10.7449208946	22.3071186178
C27	12.2548188315	10.8188820482	20.8984482810
C28	12.7257227404	11.9507405392	20.2659703875
C29	11.7770816608	9.5427800466	23.0107445578
C30	11.2580598402	9.6308146989	24.3156387256
C31	10.8176288936	8.4865670781	24.9619150529
C32	11.3705998316	7.1528816369	23.0998242441
C33	11.8213918281	8.2733861574	22.4090201627
C34	12.0112948971	3.5855618651	26.3553615924
C35	7.4217642435	6.7927387694	25.4014558888
C36	6.1817815284	7.1693722718	24.9130630635
C37	5.7858669966	6.8003220285	23.6082444321
C38	6.7103820318	6.0535181146	22.8509751664
C39	7.9446456601	5.7126775253	23.3805188868
C40	4.4920055489	7.2018315224	23.0588344630
C41	4.1804426252	7.0244903763	21.6884852305
C42	2.9742658060	7.4499845125	21.1801291702
C43	2.2963760631	8.2157416817	23.3346062210
C44	3.4944708731	7.7930610299	23.8679360798
C45	0.8417994574	8.6696495170	21.4130879278
C46	1.6211855950	10.3488372841	19.7791122710
C47	2.0297070284	11.6231259361	19.4463681083
C48	1.9959511337	12.6600132550	20.4081035313
C49	1.5513040383	12.3293573207	21.7000032233
C50	1.1523538511	11.0400056050	22.0091118826
C51	2.4266936248	14.0286822657	20.0752353688
C52	2.4887860310	14.4901961929	18.7476277061
C53	2.9396951840	15.7775151153	18.4656193292
C54	3.2636345420	16.1953315358	20.7569289963
C55	2.8261080091	14.9231897253	21.0872931378
S56	8.6996220786	12.2577954463	19.0337810218
S57	6.0611027994	13.6700553524	19.0738277565
S58	7.3070873002	10.3636138195	24.2880202263
S59	4.7292691304	11.0842871389	22.9587901630
S60	6.6771836895	14.7286647237	22.0961966886
S61	9.2997407120	13.2871120396	22.0529657133
S62	5.7311062716	9.7001003321	20.1973086521
S63	8.2757335277	8.8773350781	21.5259962613
O64	4.7798959286	13.9159854514	16.2484302893
O65	4.5798123120	16.8620685703	15.8664792157
O66	1.8465223135	17.7341873179	16.1110624782
O67	-0.2327419486	17.7141002212	18.0830265208
O68	-0.9518909093	15.1998344737	19.3829045902
O69	-1.8631337657	9.2893257351	19.9370733802
O70	-1.6189827952	6.8242043909	21.2366878419
O71	-0.6337821228	7.6653312721	23.8111703360
O72	0.2704815629	10.1138990646	24.7732713190
O73	2.5448990514	11.9278768092	25.0189694034
O74	11.1683532506	14.9144216603	24.0212266844
O75	13.9748458156	15.8295109259	23.5605784098

O76	15.4728987747	16.4142858899	21.0222212724
O77	15.5087730047	15.0889158866	18.2223509003
O78	16.1621732380	12.6342652902	19.4612476992
O79	15.2447958357	8.5049508399	23.7409578142
O80	14.3101861944	5.9635817881	24.6734203675
O81	12.7009907201	4.2402501035	23.0211560262
O82	10.1529279393	4.4043507442	21.7784154014
O83	9.8845825270	6.7591725394	19.9448208863
C84	7.5533193864	13.2695173448	19.9260746365
C85	7.6774138078	12.1372873550	17.6137746302
C86	6.4711366726	12.7508145164	17.6225621034
C87	5.4062324593	12.6415437510	16.5696714857
C88	5.6051023985	14.7340906402	15.3530498283
C89	4.7779876243	15.8667655143	14.8143188796
C90	4.0943384397	18.1439815875	15.3665983658
C91	2.6452308489	18.1138456316	14.9475842754
C92	0.4366314269	17.5018316783	15.7792545558
C93	-0.2147163046	16.8050978553	16.9409077391
C94	-1.3581792842	17.5317018305	18.9891719793
C95	-1.1080921281	16.4959408573	20.0534308131
C96	-1.2093296716	14.0463677420	20.1036277005
C97	-1.4919786031	14.0219510583	21.4618834489
C98	-1.8354561350	12.8015697603	22.0837896130
C99	-1.8699587085	11.6221901719	21.3624163251
C100	-1.5315848746	11.6231668125	19.9838559475
C101	-1.1872647721	12.8439337802	19.3266518505
C102	-0.8522480746	12.8329493435	17.9462274197
C103	-0.8709585629	11.6444648068	17.2375854166
C104	-1.2170431638	10.4239855823	17.8626529146
C105	-1.5375764327	10.4206752530	19.2104310497
C106	-2.0962967684	8.0279150308	19.2236267033
C107	-2.6519528980	7.0738391622	20.2417377051
C108	-2.1548723381	6.2767210979	22.4766665966
C109	-1.0442232320	6.2960235316	23.4953677756
C110	-1.3715238075	8.2930064949	24.9049561129
C111	-1.1606592709	9.7792176541	24.7700065769
C112	2.2456683822	10.8500459008	25.9667451603
C113	3.8805397818	12.4889157563	25.2059119925
C114	4.9651766970	11.6318332334	24.6217524261
C115	6.1339095941	11.2851271825	25.2076013869
C116	6.3031164246	10.2969257981	22.8306279017
C117	7.8146931589	13.7137633745	21.1962531393
C118	7.7387725909	14.9081644225	23.4765461770
C119	8.9283590958	14.2663949129	23.4760611109
C120	9.9450330634	14.3159416184	24.5629466488
C121	12.1803783905	15.1078840611	25.0641008547
C122	13.0997491208	16.2269606663	24.6728074471
C123	14.9835188302	16.8817263480	23.3480591861
C124	16.0337249787	16.4441111856	22.3716431380
C125	16.5204058805	16.4989483673	19.9983866518
C126	15.8846462105	16.4444430741	18.6297823991
C127	16.6523628953	14.2741820729	17.8098170996
C128	16.2821640905	12.8348839104	18.0083895218
C129	15.8658859327	11.3570236720	19.9140386707
C130	15.5649346102	10.2922277458	19.0793357892
C131	15.2401585513	9.0383874997	19.6428744557
C132	15.2192574110	8.8561808242	21.0129300632
C133	15.5322055478	9.9349952900	21.8811710718
C134	15.8658834080	11.2145105845	21.3377006275
C135	16.1818087751	12.2943049575	22.2045433505
C136	16.1404849851	12.1157468865	23.5758541618

C137	15.7978192451	10.8650225175	24.1391058755
C138	15.5250685185	9.7903151860	23.3056224624
C139	15.1566652665	8.2393796393	25.1790388636
C140	15.3158405425	6.7524092754	25.3754416349
C141	14.6395061255	5.6304395311	23.2883226578
C142	14.1602733911	4.2400044460	22.9844563690
C143	12.1402307672	3.0609151234	22.3770974509
C144	10.6404271094	3.1885520366	22.4191372897
C145	10.2610200759	4.3975356080	20.3224532618
C146	9.3170519462	5.4197523398	19.7511139020
C147	9.2166252358	7.7773424084	19.1476997529
C148	8.0451480211	8.4047639122	19.8420559363
C149	6.8772286817	8.7648713460	19.2640107078
C150	6.7185355846	9.6952020149	21.6672193839
H151	1.2988408827	21.1417920080	17.9478459958
H152	2.0258425221	21.1226278200	19.5610992377
H153	3.5848618424	22.2885667409	17.9986888008
H154	3.5542681735	20.9037870794	16.9004830753
H155	5.8805402697	17.0056970127	17.4742100076
H156	8.1646907761	16.0895796614	17.6211720410
H157	8.4405079644	17.7942173434	21.6038195563
H158	6.1625568345	18.6671977213	21.2903700077
H159	9.9805322786	15.3781507955	17.7791572436
H160	12.1868710295	14.3581572950	18.1078614810
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H186	2.3687763025	11.7970228617	18.4332566056
H187	1.4713408618	13.0718430615	22.4843659992
H188	0.8211726327	10.7554951524	23.0122795684
H189	2.1816441603	13.8665343558	17.9152302860
H190	3.0205140174	16.1599848296	17.4512207810
H191	3.5755865945	16.9027539297	21.5145638293
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H194	4.5821226077	12.0172714687	16.9317523487
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H243	16.5637367640	16.8762989049	17.8837989922
H244	14.9547492011	17.0184520990	18.6198653073
H245	16.8868505372	14.4668009786	16.7556291950
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H247	17.0549581736	12.1693001059	17.6084143362
H248	15.3246786394	12.5978883516	17.5272044681
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H259	14.1606570980	6.3580239487	22.6228928455
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H261	14.5530873300	3.5154451588	23.7112426790
H262	14.5061327416	3.9448047759	21.9837060440
H263	12.5145115421	2.9938897850	21.3445953806
H264	12.4523611407	2.1458924938	22.9009967978
H265	10.2946363139	3.2762092008	23.4550609753
H266	10.1705754732	2.3071834540	21.9610711577
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H268	9.9925196818	3.4019323718	19.9437419578
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H270	9.1935180249	5.2394533469	18.6749356953
H271	9.9841125476	8.5378579593	18.9629729914
H272	8.9034926742	7.3743094948	18.1756937839
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H275	10.7695735572	3.7789848282	28.1108970879
H276	10.6037695356	2.2213522850	27.2873954629
N277	12.0507468372	5.0626547580	26.0899538390
H278	12.8121221588	5.3098390804	25.4288501421
H279	12.2271330086	5.5698983520	26.9618333870
N280	9.5716115692	3.8642287290	26.3679880648
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H282	9.2228929084	3.1783842479	25.6932921087
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H285	5.4511820566	20.5905467526	18.2065371888
N286	2.1172159498	19.2594889158	18.5634671398
H287	1.9213378087	18.8545542481	17.6278607169
H288	1.3659732535	18.9111534316	19.1611131653
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N5	13.4490557785	13.2033419997	21.2163042013
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N10	2.9823309273	16.5903838760	19.1589249942
C11	2.0933963794	20.7166049960	18.1308429009
C12	3.4096224241	21.0960416351	17.4861429198
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C15	8.3692614859	16.7166339250	19.5375423337
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C17	6.4625768332	18.0808720696	20.1717796966
C18	9.7169329519	16.1710890769	19.8063801069
C19	10.4959543304	15.5813583328	18.7811078021

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C26	12.9010520968	10.6952496608	22.3779885849
C27	13.0278418795	10.8543758084	20.9662657818
C28	13.3093866267	12.0830457469	20.4131350505
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C35	8.0676223817	6.0417577918	23.3487793606
C36	6.7858207502	6.4221577425	22.9706076161
C37	5.8759641432	6.9492730018	23.9095639809
C38	6.3338373851	7.0557953074	25.2408391178
C39	7.6251688924	6.6561478563	25.5700647882
C40	4.5282565230	7.4026100946	23.4993057917
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C47	1.4926901023	11.6028915715	19.6808181945
C48	1.5043606078	12.7762843334	20.4931229991
C49	1.1857282291	12.5928293359	21.8636404580
C50	0.9189475790	11.3469716824	22.3844337026
C51	1.9224516899	14.0916060360	19.9879840332
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S57	-1.7570480939	14.9011622059	20.1330560714
S58	16.6017336210	12.7136337081	23.0248690535
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O67	-0.1027600631	17.5546549330	16.6658105872
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O69	9.7547069273	12.6915373083	22.3576640924
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O78	4.0984267888	11.4201499883	23.3819577075
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O80	14.4437653278	5.1812663117	23.7503937940

O81	12.4271998139	3.1669226910	23.1811044891
O82	10.2147564775	4.4745049094	21.5393810988
O83	10.2954325942	6.9702464926	19.9650208275
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C86	-1.4428582874	15.7701441315	18.6162316052
C87	5.1796374410	12.8614986903	16.7472656927
C88	5.0661538287	14.5088148402	14.9820494442
C89	4.2024690426	15.6557321249	14.5359323037
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H182	4.0420830612	8.4937606801	25.3268116565
H183	0.0551056752	8.9667906299	23.0446224639
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H185	1.1537062310	9.4649724615	19.6172151406
H186	1.6778155488	11.6484972621	18.6123542298
H187	1.1767966643	13.4152859426	22.5677491527
H188	0.7435685421	11.1824955926	23.4476898476
H189	2.4754816534	13.4962663814	17.9530520396
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H192	1.4582664762	15.2117871486	21.8179112098
H193	-1.0150978554	15.3845077193	16.5427362424
H194	4.5180561406	12.1539413778	17.2538205376
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H196	6.0412516976	14.8680443314	15.3332307596
H197	5.2165981683	13.8003645075	14.1578216358
H198	3.1660435637	15.3266866024	14.3925914981
H199	4.5825058790	16.0327264418	13.5772847608
H200	4.5485113648	18.7284888501	15.7860906654
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H202	2.5637227165	17.7012291195	13.7004775208

H203	3.1885356197	19.3599159455	13.6324101791
H204	0.2143210331	19.8836110085	15.3640045703
H205	0.6450050194	19.2111778726	13.7811555297
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H210	-2.3513746964	17.6330910513	19.1623045630
H211	-0.6061307612	17.6213229781	19.2864883523
H212	7.8469135503	11.9817891294	16.6521218066
H213	10.1622052237	11.6134085749	20.2712048336
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H221	-3.0197673502	7.3465523466	24.3427093636
H222	-2.5842144646	5.7577708748	23.6688583468
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H227	3.6641430939	13.4447493044	23.2080435470
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H231	10.7336898007	12.1826330056	24.0482981680
H232	9.0954483538	12.8634335923	24.3354134447
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H243	16.2553606394	18.0744415796	19.5228159739
H244	14.6000055886	17.5295842433	19.8678294656
H245	17.6852802665	16.2235166834	18.5479662690
H246	17.9610710469	16.0394550101	20.2937090465
H247	18.4767586999	13.9391499231	18.9874069946
H248	16.8275381096	13.9047907525	18.3935773880
H249	5.9169413016	11.3847864627	25.4132000213
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H251	8.9232966044	9.2608348831	23.1551869668
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H257	15.6189368992	4.8455976602	25.4766151349
H258	16.5367047431	5.2019446761	23.9974535475
H259	14.1918465737	4.5160197354	21.8088910919
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H261	14.1526861312	2.5602800618	24.1674428735
H262	14.0777678432	2.0440844969	22.4740099977
H263	12.2062780151	2.7065042382	21.1334345367

H264	11.6432084015	1.4524441291	22.2539958493
H265	9.8972159100	3.1818659792	23.0805931795
H266	9.6334762571	2.4590476642	21.4703527650
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H270	9.5639508214	5.6944850460	18.4665273230
H271	10.2212579498	8.9791104496	19.7875631265
H272	8.9280678277	8.1166767629	18.8776965077
H273	15.7101450754	6.4784100318	22.0939230665
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H275	10.9383411621	4.0075228517	27.9468601628
H276	10.6848450200	2.3267198468	27.4396806879
N277	12.2945526696	4.8065076268	25.7174248614
H278	12.9253275877	4.8270829276	24.8910892876
H279	12.6936110376	5.4144648233	26.4425776733
N280	9.7330082746	3.8172314685	26.2137544139
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N286	2.0086108312	19.2154540453	18.1254990250
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H291	-0.3496562565	8.4242858729	26.8503781833
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N5	13.2059724657	13.1331134592	21.3786505216
N6	11.0677432777	7.1888768769	24.4421510008
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C12	3.3917320984	21.1094932143	17.7681902896
C13	6.5140656087	17.0165792149	18.4835526971
C14	7.8032131921	16.5429541683	18.6761348344
C15	8.5417552575	16.9219137089	19.8139726655
C16	7.9211114336	17.7963246393	20.7280291362
C17	6.6297742118	18.2485946262	20.4853841499
C18	9.8944811212	16.3881840686	20.0416888446
C19	10.6425779564	15.8300542729	18.9800119084
C20	11.8653756890	15.2361266979	19.2188895882
C21	11.7169729272	15.7977771402	21.5279487672
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C24	13.2349195232	13.0208735647	22.7381626353
C25	12.8383966047	11.8395218740	23.3384398753
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C37	5.9175575936	6.9649194298	23.8323766893
C38	6.8598008206	6.3757552883	22.9675167818
C39	8.0998816919	5.9711388392	23.4414863176
C40	4.5986455422	7.3968761830	23.3431754187
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C47	1.8104784631	11.6503302954	19.6354057743
C48	1.9070362386	12.7164981594	20.5511594590
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C50	1.1615021132	11.1982265435	22.2947444876
C51	2.3863021530	14.0477045286	20.1469628217
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C53	2.7730916546	15.7656889334	18.4755180298
C54	3.4529264311	16.1456962650	20.6967525837
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S56	8.8730616259	12.4866805057	19.1008863265
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S58	7.4687683247	10.5378682987	24.3204530094
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S61	9.2830806449	13.2070969953	22.2676806310
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S63	8.4344958971	9.1808261920	21.6135476562
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O67	-0.3592719534	17.7776320405	17.7756261133
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O71	-0.6193924268	7.9623468657	24.2060570543
O72	0.3895792872	10.3759834703	25.1625644865
O73	2.7291561241	12.1483330712	25.1697998396
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O79	15.5452440827	8.1829080469	23.6372320716
O80	14.5478602809	5.5986214362	24.5048636089
O81	12.7494387065	4.0930078043	22.9011385128
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O83	10.1694796176	7.2305375793	20.0148387244
C84	7.6151072145	13.2334508983	20.0774773452
C85	7.8150133023	12.1811973805	17.7406380654
C86	6.5329210886	12.6124817521	17.8113714820
C87	5.4299429340	12.3780750849	16.8239096931
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C90	4.1828684631	17.8715634222	15.3633862572
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C95	-1.7024238547	16.7930832570	19.6014608316
C96	-1.8182041749	14.3639686784	19.8102862308
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C101	-1.8407305494	13.1001277517	19.1368815392
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C103	-1.8657839529	11.7429201196	17.1217657100
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C115	6.3216226470	11.4756288035	25.2683401774
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H169	11.0733487942	10.5129952641	24.9035839878
H170	10.2889909052	8.4120203558	25.9431188167
H171	11.9134614047	6.0930885944	22.8803752910
H172	12.7787361315	8.1405194274	21.7079473497
H173	12.0761993183	2.9019251669	25.2459376966
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H191	3.9079967007	16.8315965128	21.3995845757
H192	3.1014621506	14.6157306872	22.1280283878
H193	8.2347278590	11.6594611660	16.8871105272
H194	4.6646357131	11.7262901567	17.2594442277
H195	5.8225578299	11.8889109513	15.9238762309
H196	6.3854533004	14.7962118395	15.9171845025
H197	5.7265731720	13.7306069140	14.6519789731
H198	3.5600184015	15.1276990929	14.8096493149
H199	4.9775456004	15.8763069410	14.0329060972
H200	4.3316826902	18.5950607789	16.1719425871
H201	4.8728528625	18.1161772049	14.5435529031
H202	2.6042112290	17.1782466842	14.0451058111
H203	2.5325873291	18.9029427310	14.4473176028
H204	0.0728442274	18.4320571011	15.2496306463
H205	0.4329958478	16.7920134993	14.6496213712
H206	0.1114207641	15.8899030191	16.9785463958
H207	-1.3471345947	16.6430624083	16.3038530573
H208	-1.6918532805	18.8147619262	18.9367691709
H209	-2.4585869154	17.6908313716	17.7952897357
H210	-2.6212596457	16.9324194462	20.1840216175
H211	-0.8389922632	16.8624643546	20.2741317142
H212	-1.9223469359	15.4083274808	21.6962587622
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H214	-1.7389705758	13.8915657174	17.1254303936
H215	-1.8511762850	11.6623831939	16.0391105633
H216	-2.0070336071	9.5999949656	17.3944535451
H217	-3.2282618939	8.3729075058	18.8425727156
H218	-1.5566220253	7.8087782584	19.0985755633
H219	-3.2956088247	6.4664465221	20.3761121915
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H221	-3.0927428542	7.2850054127	23.3472403495
H222	-2.6774335635	5.6539041112	22.7788731789
H223	-0.2544487242	6.1169448046	23.3947822261
H224	-1.3529778874	6.0747258112	24.7910066988
H225	2.8531816892	10.2612082024	26.1217475865
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H227	4.0380583549	13.6525099716	24.7668293953
H228	4.2995786071	12.9174672256	26.3594858060
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H230	7.2419165141	15.3024579992	24.5239477555
H231	10.0238316694	13.0730876989	25.1796541963
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H241	16.8922066990	17.6932585582	20.6592060092
H242	17.1024051086	15.9300132737	20.6858946160
H243	16.4665821487	17.1164822062	18.4053297319

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H246	17.4717408569	14.7285569847	18.9292285648
H247	17.0587516077	12.4721401729	17.8754998744
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H255	16.3022433481	8.3025660155	25.6063220827
H256	14.5261986582	8.2068757536	25.4653275180
H257	15.5333167045	6.0681382382	26.2454281119
H258	16.5781317468	6.0005999977	24.8129767556
H259	14.4940861288	5.9971704628	22.4440278476
H260	15.9409246305	5.1267441719	23.0055888746
H261	14.5028613044	3.1319493291	23.5550286237
H262	14.4784698382	3.5635275866	21.8264796582
H263	12.3859998955	2.9464625759	21.1860652980
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H265	10.1977488570	3.4381449947	23.2952071358
H266	9.9726050022	2.6227876375	21.7233292764
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H268	10.3922116276	3.8853715328	19.7930538025
H269	8.6406049945	5.7630266782	20.0318144594
H270	9.6857223763	5.7750356550	18.5900874863
H271	10.2383418077	9.0752187724	19.1526757233
H272	9.2779047567	7.9141399031	18.2211303204
H273	6.8398220711	8.8611943082	18.2870124751
C274	10.8884347336	3.1345015542	27.0489435833
H275	10.9655705613	3.6140363219	28.0278106028
H276	10.7141582444	2.0676384254	27.2031400794
N277	12.2136740672	4.8691020680	25.9758152214
H278	12.9543892918	5.0846736623	25.2814331253
H279	12.4623627876	5.3522073608	26.8442410306
N280	9.7052583537	3.7514541176	26.3318402069
H281	8.9458570760	3.9228142557	26.9949726370
H282	9.3348405552	3.0937556915	25.6403186885
N283	4.5088957075	20.4743997610	18.5650078663
H284	4.6266204630	20.9691673479	19.4543050187
H285	5.3957837824	20.5659133921	18.0636599841
N286	2.1117893156	19.1253495428	18.3773890831
H287	1.9496741649	18.7119866217	17.4373760669
H288	1.3531894934	18.7587191285	18.9559597792
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H291	-0.8261025959	8.1876225411	26.2803812692
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H296	0.6097723085	10.5540514376	27.2465177497

$\mathbf{7}_{out}^{9+}$	X	Y	Z

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Pt2	10.3714081846	5.5965925854	25.1121159191
N3	5.8806261429	17.7889155214	19.2234959302
N4	12.4115256923	15.2443541913	20.3766183314
N5	13.5365536265	13.2600219493	21.2245046038
N6	11.2332729334	7.2346328012	24.1634918465
N7	8.4374239746	6.1846380066	24.5873917589
N8	1.9764115832	8.3492869916	22.5645563486
N9	0.8699235287	10.2588169253	21.5301861693
N10	3.1200157559	16.6210952290	19.3058764689
C11	2.1403388767	20.6684978496	17.9376856843
C12	3.5025087525	21.0121243490	17.3747669819
C13	6.4493825058	16.8789119414	18.3812080098
C14	7.7487724142	16.4233778268	18.5711510243
C15	8.5151855183	16.8702156394	19.6670225422
C16	7.9102466220	17.8123801577	20.5255027323
C17	6.6114416910	18.2519972805	20.2788894494
C18	9.8756151620	16.3374541830	19.9134059192
C19	10.6561760779	15.8082968410	18.8576137411
C20	11.9048121126	15.2702493562	19.1028146202
C21	11.7081444668	15.7828331565	21.4208665064
C22	10.4486389649	16.3189509509	21.2055594667
C23	13.7331491485	14.6026158640	20.6457680043
C24	13.5525562119	13.1069844020	22.5916361512
C25	13.2851623834	11.8766171527	23.1525979641
C26	12.9323477396	10.7572578380	22.3577921844
C27	13.0219920278	10.9355889470	20.9503352030
C28	13.3269743601	12.1661210331	20.4103990117
C29	12.4216901668	9.5177133632	22.9717760668
C30	12.0949614107	9.4776014366	24.3520291525
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C34	12.1542549604	3.5359114218	26.2868192920
C35	8.0665005312	6.1905787763	23.2745208815
C36	6.7846867316	6.5616581922	22.8855896904
C37	5.8264471395	6.9627419890	23.8392565217
C38	6.2301241978	6.9443477317	25.1926667234
C39	7.5227125903	6.5562945193	25.5307645526
C40	4.4792372349	7.4146799739	23.4208604196
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C43	2.4316241615	8.6807377670	23.8168679283
C44	3.6672747096	8.2257401579	24.2489019256
C45	0.6695359708	8.9016475092	22.0909222616
C46	1.1582200267	10.4301585341	20.1909446682
C47	1.4850495670	11.6762790880	19.6989173318
C48	1.5279897934	12.8155141044	20.5520010954
C49	1.1382926824	12.6032223369	21.8951736036
C50	0.8342803719	11.3434300010	22.3723089380
C51	2.0186552157	14.1321278473	20.0971807117
C52	2.3761769457	14.3999185519	18.7584667215
C53	2.9173639616	15.6315326169	18.3900212719
C54	2.7505678110	16.4003991494	20.6040454422
C55	2.2012364371	15.1956979136	21.0169521414
S56	-1.8069287878	12.7921464390	17.4478298396
S57	-2.1125178865	14.4358426217	19.8764256594
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O65	4.1351849933	16.6004201347	15.6442256837
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O67	0.1607574945	17.0159613143	16.7177578526
O68	5.9724033011	13.6753758019	18.0889369809
O69	9.9005041742	12.8870052510	22.6041528652
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O71	-0.5457885105	8.2117382968	24.6805610885
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O73	2.5383096511	12.6081498327	24.6791284589
O74	10.8427271244	14.4656545798	23.9999726638
O75	13.2946078451	15.8821238457	24.3590667893
O76	15.3336077430	16.4935637589	22.3423873703
O77	16.1763073873	15.9437962380	19.6616957948
O78	4.1110708100	11.4895703043	23.3287910657
O79	8.7538311809	8.4386253802	20.9708781298
O80	14.2709078694	5.2482555849	23.4469952739
O81	12.2207407155	3.0282047729	23.2568172495
O82	10.3457315311	4.6498954438	21.4852065645
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C85	-1.5057204616	14.4947949059	17.3027762240
C86	-1.6430628133	15.2800120870	18.4042229039
C87	5.2239528750	12.8895215894	17.0883755741
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C89	4.2405187588	15.5000526573	14.6772056811
C90	4.3409442008	17.9309995814	15.0727991925
C91	3.1364287643	18.4842151736	14.3454398067
C92	0.7222817248	18.5219095746	14.8341535885
C93	0.3476102720	17.1179517395	15.2628926634
C94	-1.1704702793	17.4458006017	17.1639204735
C95	-1.4673025249	16.7734329836	18.4934283472
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C97	8.0391646046	12.3520531516	17.9974151443
C98	9.1915826148	11.8815822412	18.6687129223
C99	9.4167124222	12.1920690774	19.9971445995
C100	8.4915708909	13.0025517926	20.7053897674
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C103	6.6437666727	14.6433820474	22.0799407542
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C109	-0.9795206647	6.8171927584	24.5450380726
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C127	17.6096915632	15.7554183403	19.4426960970
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H168	13.3977797436	12.3340611547	19.3409296235
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H177	5.5494370965	7.2017750991	25.9989876148
H178	7.8521010239	6.5379685569	26.5642544412
H179	4.4729409994	6.3852754870	21.4885124211
H180	2.2727089794	7.2534639295	20.7961608022
H181	1.7637607388	9.2868671693	24.4325102573
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H188	0.6197043848	11.1580307481	23.4280800096
H189	2.2579509249	13.6637858281	17.9719653679
H190	3.2089149205	15.8519674638	17.3659568404
H191	2.9058869583	17.2177029798	21.2979558664
H192	1.9335083896	15.1062311119	22.0646972798
H193	-1.2268915162	14.8573732792	16.3208277282
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H197	5.3496760903	13.6751350820	14.4608128688
H198	3.2395282987	15.0965750371	14.4832556221
H199	4.6512766562	15.8704196496	13.7309366182
H200	4.5950435154	18.5578039321	15.9336461883
H201	5.2055613066	17.9123215769	14.3938799014
H202	2.7469141741	17.7595993563	13.6172243278
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H205	0.6634956368	18.6332356073	13.7424464295
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H208	-1.2032868121	18.5392829908	17.2869808895
H209	-1.9215528607	17.1719560563	16.4072096723
H210	-2.3790391907	17.2258337004	18.9086537168
H211	-0.6639625644	17.0044237081	19.2100537427
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H214	5.4691047906	14.5906411270	20.2717048701
H215	5.9504710425	15.2822371552	22.6248017361
H216	8.0370958705	14.5739458080	23.7398253806
H217	-4.3032814875	7.6305424710	19.9164148388
H218	-2.5802458312	7.2982240668	19.9121355393
H219	-3.7488949663	6.0319108611	21.6802564252
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H221	-3.1110504772	7.2574104074	24.4675571836
H222	-2.6458695549	5.6467192520	23.8762157756
H223	-0.2254655094	6.3379062554	23.9110281731
H224	-0.9727163081	6.3267775044	25.5274033727
H225	3.0923124170	10.8729366958	25.7368247343
H226	3.1121349550	12.3825279144	26.6979072226
H227	3.6418036447	13.5081584245	23.2596312604
H228	4.6003619165	13.0222842815	24.7096296598
H229	17.5977547448	14.7765704470	22.0432074292
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H231	10.9076604491	12.3851320916	24.2801381783
H232	9.3161963311	13.1511631654	24.6048682612
H233	10.5534616598	14.8877960699	26.0510060796
H234	12.0489255437	13.9926141230	25.6623833920
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H236	11.4865693199	16.8839324769	24.7917272184
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H240	15.8366357646	15.5613314885	24.1282850718
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H242	17.1673618201	17.3800866451	21.8227680133
H243	16.3295138768	18.0483882951	19.5185831542
H244	14.7388160729	17.3730738619	19.9214417002

H245	17.9288315432	16.3353321921	18.5675647963
H246	18.1867864107	16.1123976702	20.3090267125
H247	18.8877064375	14.1032091527	18.9580538864
H248	17.2640546538	13.9690140049	18.3029966615
H249	5.8925365466	11.4296488006	25.4066767531
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H252	4.0740049418	10.9113841620	20.9976755728
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H258	16.3723738197	5.0509714570	23.5443618043
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H261	14.0923601200	2.6812669688	24.0748183547
H262	13.8979662310	1.9951722577	22.4565707664
H263	12.0277704951	2.5743009176	21.2009857703
H264	11.2154462559	1.4514304840	22.3037525374
H265	9.7143539891	3.4428118349	22.9969740982
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H270	9.6657185281	5.8916381877	18.4168634773
H271	10.3428934856	9.1387624686	19.8266303988
H272	9.0514574769	8.3263284332	18.8740958650
H273	15.7646188606	6.4537728074	21.6911374237
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H276	10.7040118556	2.4833985227	27.5088647560
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H282	9.5212472245	3.1202067212	25.5461170661
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H285	5.4789345105	20.4610892639	17.8328407071
N286	2.0817387671	19.1792862362	18.1685785361
H287	1.8891329528	18.6950111119	17.2722518821
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C12	3.3860681356	21.1698757670	17.2273831347
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C14	7.8043373246	16.7889200714	18.4660666712
C15	8.5183026700	17.2072461975	19.5988434819
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C18	9.8248505262	16.6203184276	19.9106731453
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C20	11.7551047786	15.3245971074	19.2437504084
C21	11.4820243569	15.9298504425	21.5358491762
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C24	12.3594798470	13.0290875257	22.7581754020
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C27	12.2693924460	10.7972151257	21.1240012835
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C31	11.1563123986	7.9882655980	25.0193345946
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C34	12.0949227418	3.3045581581	26.1898520738
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C36	6.6670999676	5.9742674315	22.7770383970
C37	5.6498535290	6.2840444937	23.6899561282
C38	5.9285490465	6.1417389163	25.0610233752
C39	7.2034345707	5.7814961801	25.4690826340
C40	4.3924022721	6.8693271284	23.2194787113
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C47	2.1058797771	11.8156111622	19.5421599552
C48	2.2815241648	12.8754087080	20.4554107373
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C51	2.6169990700	14.2277036861	19.9986163060
C52	3.1855695463	14.4643720064	18.7356763249
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C54	2.7486568729	16.6115201156	20.3944039583
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O68	-0.9949163224	15.1670820643	19.4226412698
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O70	-1.3142975087	7.1668285925	22.4153155136
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O72	1.2822010154	10.7799618534	25.2404771819
O73	3.8153800332	12.2153077341	25.3752770452
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O77	15.3150666304	15.5289093542	19.1551870242
O78	16.0617390438	12.9875715493	20.0839366407
O79	15.2267062516	8.2778283487	23.7192610083
O80	14.1837801592	5.6663261552	24.3436204329
O81	12.3032776020	4.3372089461	22.4763905911
O82	9.7552360122	4.6393136701	21.0569665440
O83	9.3660135726	6.8382356373	18.9632850250
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C85	8.6230746015	12.0602575283	17.8898382560
C86	7.4128984218	12.5233822109	17.4905894417
C87	6.6768202702	12.3065117690	16.1983768017
C88	6.4913332417	14.5215319127	15.1797503948
C89	5.4830368578	15.4774117043	14.6042366697
C90	4.3604607133	17.5959466973	15.1347328182
C91	2.9125148406	17.4263662272	14.7553322887
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C93	0.0720771764	16.3503657224	16.9251454309
C94	-1.3768053667	17.3885318049	18.6108297495
C95	-1.2213585464	16.5628207996	19.8605071359
C96	-1.1859987904	14.1424552466	20.3063809831
C97	-1.3462055085	14.3211436731	21.6836569233
C98	-1.5932010352	13.2092443136	22.5016579203
C99	-1.6814547054	11.9259521200	21.9618679174
C100	-1.4977866219	11.7241178280	20.5758018234
C101	-1.2300050171	12.8353732873	19.7154232125
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C120	8.6984389923	15.1194201556	24.7566864654
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C127	16.5620812519	14.8868745062	18.7381357660

C128	16.3236700052	13.4097216820	18.6870192663
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H229	7.5509497973	10.7815250979	25.9476737361
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C37	5.7501484358	6.5507297209	23.8849050773
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C47	1.9292711062	11.6522473516	20.1984797792
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C50	1.3837911096	11.4508010507	22.9074700181
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O77	20.1936220294	12.2970787527	23.4570037190
O78	4.5526316308	10.9578387504	24.0623646776
O79	9.0409129168	8.5298702306	20.8203483614
O80	16.4779331067	3.7846207962	23.5789587336
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H234	11.9357407684	13.3927616509	25.8706259277
H235	12.9389065453	15.7002432057	26.1893271251
H236	12.4032392336	16.1170524332	24.5504722698
H237	15.3999228569	15.9203082210	24.0458370035
H238	14.9334376538	16.0375007938	25.7548124932
H239	16.9514172181	14.9533943413	25.9592873667
H240	15.8510444290	13.5612144591	25.9048306289
H241	18.7655622349	14.0617263115	25.1502488482

H242	18.0900850097	12.4188553327	25.0697308571
H243	19.2398110750	14.0179011643	22.7048907161
H244	18.3792921056	12.4619933685	22.5546247780
H245	21.5121630731	13.9147555766	23.7525066482
H246	20.8205046026	13.2254955774	25.2441828050
H247	23.1472125545	12.4821726279	25.0181440080
H248	22.8589210762	11.8996545244	23.3800914117
H249	6.5154355104	10.6481645095	25.9081189677
H250	8.7607313826	9.7129284732	25.4413069478
H251	9.3619865733	8.9793788932	23.1305349234
H252	4.2475395890	10.6008604383	21.6952653043
H253	4.8183827817	9.7584506383	19.4120654112
H254	7.0197476814	8.7759189659	18.9527454859
H255	18.8631149496	3.0672524512	25.8309987599
H256	17.4521949662	4.0910250211	26.0312090215
H257	16.9808401976	2.0599949395	24.6954198574
H258	18.1707075299	2.5445908901	23.4699714462
H259	15.4502332917	3.9616584707	21.8197562484
H260	16.5974947002	2.6049232619	21.8500894710
H261	14.6938727207	2.0923493448	23.9332048235
H262	14.7803828361	1.2241958233	22.3897756676
H263	13.3799534325	2.6901525745	20.3948059555
H264	13.0127386371	1.1571925013	21.2193177966
H265	10.8523578130	2.3310905193	22.0776552065
H266	10.9471986172	1.7999876190	20.3864797583
H267	9.8185735824	3.1881774173	19.1553975626
H268	8.9958960890	3.8015586272	20.6058878013
H269	9.0095199069	5.2996945521	18.4708247301
H270	10.7253789312	5.5986840632	18.8490653390
H271	10.3794482513	7.9145134561	19.4170204238
H272	8.6759323487	7.7274748304	18.9005134399
H273	18.6437665472	4.7149628812	22.6142053293
C274	10.3981781349	2.0284348320	25.9790422394
H275	10.5576709724	2.5137049677	26.9445179555
H276	10.0729119557	1.0010391269	26.1588543629
N277	11.9462093064	3.5132715103	24.7718141338
H278	12.5053205462	3.5027137613	23.8955801173
H279	12.4912426710	3.9573717024	25.5164709164
N280	9.3155053827	2.7936641150	25.2571367095
H281	8.5224967055	2.9567006298	25.8817974200
H282	8.9500301112	2.2367380036	24.4785572274
N283	4.8408999101	20.1452712697	17.8687246046
H284	5.1070743915	20.7650472239	18.6399553904
H285	5.6462656117	20.1025153015	17.2396534074
N286	2.3733709256	18.9739582083	18.3525777536
H287	1.9126406510	18.4056155039	17.6111306763
H288	1.8263264873	18.8565943731	19.2092148151
H289	9.8647965466	10.6822811873	18.3015985210
H290	-2.5705022242	9.6831200026	25.9517648443
H291	-1.1403164298	8.7314166541	25.5048951169
H292	-1.1188702724	11.7084686568	26.2579721867
H293	-0.8112559194	10.3811673857	27.4048774250
C294	1.4609735736	11.4244425137	26.9084108858
H295	1.0880673367	12.4561841276	26.9387474438
H296	1.3346925993	10.9836863303	27.9058907439

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